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Orbit spaces of reflection groups with 2, 3 and 4 basic polynomial invariants*

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Abstract. Functions which are covariant or invariant under the transformations of a compact linear group can be expressed advantageously in terms of functions defined in the orbit space of the group, i.e. as functions of a finite set of basic invariant polynomials. The equalities and inequalities defining the orbit spaces of all finite coregular real linear groups (most of which are crystallographic groups) with at most four independent basic invariants are determined. For each group G acting in the Euclidean space $\mathbb{R}^n$, the results are obtained through the computation of a metric matrix $\hat{P}(p)$, which is defined only in terms of the scalar products between the gradients of a set of basic polynomial invariants $p_1(x), \ldots p_q(x)$, $x \in \mathbb{R}^n$ of G; the semi-positivity conditions $\hat{P}(p) \geqslant 0$ are known to determine all the equalities and inequalities defining the orbit space $\mathbb{R}^n/G$ of G as a semi-algebraic variety in the space $\mathbb{R}^q$ spanned by the variables $p_1, \ldots, p_q$. In a recent paper, the $\hat{P}$-matrices, for $q \leqslant 4$, have been determined in an alternative way, as solutions of a universal differential equation; the present paper yields a partial, but significant, check on the correctness and completeness of these solutions. Our results can be easily exploited, in many physical contexts where the study of covariant or invariant functions is important, for instance in the determination of patterns of spontaneous symmetry breaking, in the analysis of phase spaces and structural phase transitions (Landau's theory), in covariant bifurcation theory, in crystal field theory and in most areas of solid-state theory where use is made of symmetry adapted functions.

1. Introduction

Functions which are covariant or invariant under the transformations of a compact linear group (hereafter abbreviated as CLG) G play an important role in physics, and the determination of their properties is often a basic problem to solve.

An example, which is relevant both to elementary particle and solid-state physics, is offered by the determination of the possible patterns of spontaneous symmetry breaking in theories in which the ground state of the system is determined by the minimum of an invariant potential $V(x)$.

Let us sketch the relevant physical context. The symmetry group G of the formalism used to describe a physical system acts as a permutation group on the set of the solutions of the evolution equations. When the ground state of the system is invariant only with respect

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to a proper subgroup $G_0 \subset G$, the G-symmetry is said to be *spontaneously broken* (see, for instance [1–4] and references therein) and G_0 turns out to be the *true* symmetry group of the system [5].

One of the most common classical mechanisms of spontaneous symmetry breaking can be formalized in the following way. The ground state is represented by a vector x_0 belonging to the Euclidean space $\mathbb{R}^n$, on which G acts as a group of linear transformations; x_0 is determined as the point at which a G-invariant potential $V(x)$ assumes its absolute minimum (V might be a Higgs potential in a gauge field theory or a thermodynamic potential in a Landau theory of structural phase transitions), and G_0 is the isotropy subgroup of G at x_0 (the little group of G_0). Generally, the potential also depends on parameters γ (for instance scalar self-couplings in Higgs potentials, or pressure and temperature in thermodynamic potentials), that cannot be determined from invariance requirements under transformations of G. In this case x_0 and G_0 can depend on the γ's, and various patterns of spontaneous symmetry breaking are allowed, corresponding to distinct structural *phases* of the system.

In supersymmetric field theories the absolute minimum of the potential controls both the spontaneous symmetry and supersymmetry breaking (see, for instance [6] and references therein), and often the features of the two breaking schemes are related [7].

In all the cases just mentioned, the determination of the ground state of the system rests on a precise determination of the point x_0, where the potential takes on its absolute minimum, and the determination has to be analytical, since the isotropy subgroups of G at nearby points may be different.

Even if trivial in principle, the analytical determination of the minimum of an invariant potential is generally a difficult computational task (even if one uses polynomial approximations for the potential), owing to the large number n of the variables x_i which are often involved. An additional difficulty is related to the degeneracy of the stationary points of the potential, which is an unavoidable consequence of the invariance properties of the potential; In fact, it prevents a direct application [8] of Morse's theory [9]. Also the use of an extended Morse theory [10] seems not to give large advantages [11].

In 1971, Gufan [12, 13] proposed a new, more economical, approach to the problem, which was based on the remark that a G-invariant function $V(x)$ can be expressed as a function $\hat{V}(p_1, \ldots, p_q)$ of a finite set $p(x) = (p_1(x), \ldots, p_q(x))$ of basic polynomial invariants. When the point $p \in \mathbb{R}^q$ is in the domain spanned by $p(x),\ x \in \mathbb{R}^n$, the function $\hat{V}(p)$ has the same range as $V(x)$, but is not plagued by the same degeneracies. Gufan's proposal found immediate applications in crystal field theory (see [14–19], to cite but a few of the pioneering papers on the subject). A full and correct exploitation of his idea required, however, an exact determination of the ranges of the functions $p_i(x)$, a non-trivial problem that was only solved ten years later, when it was independently remarked [20] that any G-invariant function, being a constant along each orbit of G, can be considered a function in the orbit space $\mathbb{R}^n/G$ of the action of G in $\mathbb{R}^n$. As a consequence, the problem of determining the stationary points of $V(x)$ could be more economically reformulated in $\mathbb{R}^n/G$ [21], where the p_i's can be used advantageously to parametrize the orbits. In $\mathbb{R}^n/G$, the images of all the points of $\mathbb{R}^n$ with the same invariance properties under G transformations form smooth sub-manifolds, which are usually called *strata*. By varying the parameters γ, the location of the minimum of $V(x;\gamma)$ may shift to a different stratum, thus causing a (structural) phase transition of the system.

A sensible progress in the characterization of the geometry of the orbit spaces of the CLGs was achieved using the powerful tools of geometric invariant theory [22, 23], which led to the discovery of a simple recipe allowing us to build a concrete image of the orbit space of any linear CLG and its stratification [20, 21, 24, 25]. It was shown that the orbit spaces of the CLGs are connected semi-algebraic varieties, whose defining equations and inequalities can be expressed in the form of positivity conditions of matrices $\hat{P}(p)$ built only in terms of the gradients of the basic polynomial invariants $p_1(x), \dots, p_q(x)$:

$$\hat{P}_{ab}(p(x)) = \sum_1^n{}_i \frac{\partial p_a(x)}{\partial x_i}\frac{\partial p_b(x)}{\partial x_i} \qquad a, b = 1, \dots q\, . \tag{1}$$

Using this result, one can obtain, for instance, a concrete realization of the orbit space of any *coregular*† finite linear group. In fact, the class of these groups has been shown to coincide with the class formed by the finite groups generated by reflections (which are almost all crystallographic groups) and explicit or algorithmic descriptions of their basic polynomial invariants have been given by many authors (see for instance [26–32]).

For a general CLG, the matter is not that simple, since the determination of a minimal complete set of basic invariant polynomials, i.e. of a minimal integrity basis of the ring of polynomial invariants of G, may be a difficult problem to solve‡. This serious handicap in the direct approach to the determination of the $\hat{P}$-matrix associated to a general CLG stimulated the research, and led to the discovery, of an alternative indirect method of computation of the $\hat{P}$-matrices associated to CLGs. These matrices have been shown [36–38] to be solutions of a *master* differential equation, satisfying convenient initial conditions (*allowable solutions*). The master equation assumes a particularly simple canonical form (*canonical equation*) for compact coregular linear groups (hereafter abbreviated as CCLGs). The form of the canonical equation is the same for all CCLGs; it does involve only the degrees of the elements of the integrity bases as free parameters.

The master equation approach to the determination and classification of the $\hat{P}$-matrices gives strong support to the conjecture that the orbit spaces of all the compact linear groups possessing a basis of q independent basic polynomial invariants with the same degrees can be classified in a finite (and small, for small dimensions and degrees) number of isomorphism classes. The conjecture has been proved to hold true for $q \leqslant 4$.

This fact makes the orbit-space approach to the study of covariant functions, and, in particular, of spontaneous symmetry breaking, particularly appealing. In fact, invariance properties are often the only bounds which are imposed on the potential (beyond regularity and stability properties and/or bounds on the degree, when the potential is a polynomial function). If the symmetry groups of the potentials of different theories share isomorphic orbit spaces, the potentials have the same formal expression and the same domain when written as functions in orbit space, despite the completely different physical meaning of the variables and parameters involved in the definition of the potentials. Thus, the problems of determining the geometric features of the phase space, the location and stability properties of the minima of the potential, the number of primary strata (and, consequently, the maximum number of phases) and the allowed transitions between primary strata are identical in all these theories [21, 35–37].

The pursuit of the ambitious program of determining the orbit spaces of all the CLGs, following the master equation approach, has already given encouraging results, but has left some serious open problems [38]. The main ones are listed below; some of them will be dealt with and partially solved in this paper:

(i) All the allowable solutions of the canonical equation have been determined for $q \leqslant 4$ (see [37, 39] hereafter referred to as I and II), while for $q > 4$, the determination of all

† G is said to be coregular if there is no algebraic relation among the elements of a minimal set of its basic invariant polynomials, i.e. among the elements of the minimal integrity bases of the ring of its polynomial invariants.

‡ A complete classification of compact coregular linear groups is known, at present, only for finite groups and for simple [33] and semisimple [34] Lie groups.

the allowable solutions appears to be still possible, but extremely lengthy. The set-up of an inductive procedure for the determination of at least a part of the allowable solutions of the canonical equation is in progress [40, 41].

(ii) The canonical equation and the associated initial conditions are only a set of necessary conditions that the $\hat{P}$-matrices of the CLGs must satisfy; even if quite stringent, they need not be sufficient. Therefore, once the allowable solutions of the canonical equation have been determined, the problem remains of selecting those which are really generated by a group. In this paper we shall give a partial answer to this problem in the case of coregular groups with $q \leqslant 4$.

(iii) An effective formalization of the condition that there is no algebraic relation among the elements of a minimal integrity basis (minimality + regularity condition) has not yet been found, nor used, in I and II. Thus, it cannot be excluded that some of the allowable $\hat{P}$-matrices determined in I and II are indeed associated to non-minimal bases or to non-coregular groups.

(iv) A sound analysis of the structure of the master equation in the general non-coregular case is still missing; some results have been obtained only for non-coregular CLGs with a sole independent relation among the elements of the minimal integrity bases [42].

The paper will be organized in the following way. We shall begin, in section 2, with a short survey of the geometry of linear group actions, of the properties of the canonical equation, and we shall briefly argue on the possibility of classifying the orbit spaces of the CCLGs through the determination of the allowable solutions of the canonical equation. In sections 3 and 4 we shall determine explicitly the $\hat{P}$-matrices associated to all the finite irreducible and, respectively, reducible reflection groups with no more than four independent basic invariants. The results will be obtained using the explicit form of the basic invariant polynomials of the reflection groups that can be found in the mathematical and physical literature. A comparison of our results with the allowable solutions of the canonical equation reported in I and II will allow us to identify generating groups for all the irreducible, and some of the reducible, allowable $\hat{P}$-matrices.

After a few concluding remarks on our mathematical results, collected in section 5, in the last section we shall illustrate how they can be used in one of the specific physical contexts mentioned in the introduction. Our aim will be to show that, despite the sophisticated mathematical tools that have been used to achieve the results presented in the paper, their practical exploitation in physical contexts only requires an elementary use of standard analysis, geometry and group theory. The physical problem we shall deal with in section 6 has been studied by various authors in the past [53]; our revisitation will not lead to essentially new results, but to the fact that explicit knowledge of the algebraic relations defining the strata will allow us to arrive at explicit analytic solutions in a particularly simple way.

2. An overview of the geometry of linear group actions

In this section, we shall first define most of our notation and recall, without proof, some results concerning invariant theory and the geometry of orbit spaces of CLGs (see for instance [43, 44] and references therein), then we shall introduce the first definitions and the basic tools for our subsequent analysis.

For our purposes, it will not be restrictive to assume that G is a matrix subgroup of $O_n(\mathbb{R})$† acting linearly in the Euclidean space $\mathbb{R}^n$.

† The stronger assumption $G \subseteq SO_n(\mathbb{R})$ introduced in I and II is due to a slip; in fact, the unimodularity condition has never been used in these references.

2.1. Orbits and strata

We shall denote by $x = (x_1, \dots, x_n)$ a point of $\mathbb{R}^n$. The group G acts in $\mathbb{R}^n$ in the following way:

$$x'_i = (g \cdot x)_i = \sum_1^n {}_j g_{ij} x_j \qquad x \in \mathbb{R}^n \qquad g \in G\,. \tag{2}$$

The G-orbit $\Omega_{\bar{x}}$ through $\bar{x} \in \mathbb{R}^n$ and the *isotropy subgroup* $G_{\bar{x}}$ of G at $\bar{x} \in \mathbb{R}^n$ are defined by the following relations:

$$\Omega_{\bar{x}} = \{g \cdot \bar{x} \mid g \in G\} \qquad G_{\bar{x}} = \{g \in G \mid g \cdot \bar{x} = \bar{x}\}\,. \tag{3}$$

The invariance of the Euclidean norm under orthogonal transformations assures that the G-orbit through $\bar{x}$ is contained in the sphere of radius $\bar{x}$, centred in the origin of $\mathbb{R}^n$, while the linearity of the action of G in $\mathbb{R}^n$ implies

$$G_{\bar{x}} = G_{\lambda \bar{x}} \qquad \forall \lambda \in \mathbb{R}_*\,. \tag{4}$$

The isotropy subgroup of G at the origin of $\mathbb{R}^n$ coincides with G. The isotropy subgroups $G_{g \cdot \bar{x}}$ of G, at points lying on the same orbit $\Omega_{\bar{x}}$ are conjugated subgroups in G:

$$G_{g \cdot \bar{x}} = g G_{\bar{x}} g^{-1} \qquad \forall g \in G\,. \tag{5}$$

The class of all the subgroups of G conjugated to $G_{\bar{x}}$ in G will be said to be the *orbit type of* $\Omega_{\bar{x}}$ or, equivalently, of the points of $\Omega_{\bar{x}}$; it specifies the symmetry properties of $\Omega_{\bar{x}}$ under transformations induced by elements of G.

The set of all the points $x \in \mathbb{R}^n$ (or, equivalently, of all the orbits of G) with the same orbit type form an *isotropy-type stratum of the action of* G *in* $\mathbb{R}^n$, hereafter called simply a *stratum of* $\mathbb{R}^n$. All the connected components of a stratum are smooth iso-dimensional sub-manifolds of $\mathbb{R}^n$.

2.2. The orbit space

The *orbit space* of the action of G in $\mathbb{R}^n$ is defined as the quotient space $\mathbb{R}^n/G$ (obtained through the equivalence relation between points belonging to the same orbit) endowed with the quotient topology and differentiable structure. We shall denote by π the canonical projection $\mathbb{R}^n \to \mathbb{R}^n/G$. Whole orbits of G are mapped by π into single points of $\mathbb{R}^n/G$. The image through π of a stratum of $\mathbb{R}^n$ will be called an (*isotropy-type*) *stratum of* $\mathbb{R}^n/G$; all its connected components turn out to be smooth iso-dimensional manifolds.

Almost all the points of $\mathbb{R}^n/G$ belong to a unique stratum Σ_p, the *principal stratum*, which is a connected open dense subset of $\mathbb{R}^n/G$. The boundary $\overline{\Sigma_p} \backslash \Sigma_p$ of Σ_p is the union of disjoint *singular* strata. All the strata lying on the boundary $\bar{\Sigma} \backslash \Sigma$ of a stratum Σ of $\mathbb{R}^n/G$ are open in $\bar{\Sigma} \backslash \Sigma$.

The following partial ordering can be introduced in the set of all the orbit types: $[H] < [K]$ if H is a subgroup of a subgroup of G conjugated with K. The orbit type $[H]$ of a stratum Σ is contained in the orbit types $[H_b]$ of all the strata Σ_b lying in its boundary; therefore, more peripheral strata of $\mathbb{R}^n/G$ are formed by orbits with higher symmetry under G transformations. The number of distinct orbit types of G is finite and there is a unique minimum orbit type, the *principal orbit type*, corresponding to the principal stratum; there is also a unique maximum orbit type $[G]$, corresponding to the image through π of all the points of $\mathbb{R}^n$, which are invariant under G.

A faithful image of $\mathbb{R}^n/G$ can be obtained making use of a basic result of the geometric approach to invariant theory in the following way.

A function $f(x)$ is said to be G-invariant if

$$f(g \cdot x) = f(x) \qquad \forall x \in \mathbb{R}^n \qquad g \in G\,. \tag{6}$$

The set of all real, G-invariant, polynomial functions of x forms a ring $\mathbb{R}[x]^G$, that admits a finite integrity basis [45, 46]. Therefore, there exists a finite minimal collection of invariant polynomials $p(x) = (p_1(x), p_2(x), \ldots, p_q(x))$ such that any element $F \in \mathbb{R}[x]^G$ can be expressed as a polynomial function $\hat{F}$ of $p(x)$:

$$\hat{F}(p(x)) = F(x) \qquad \forall x \in \mathbb{R}^n\,. \tag{7}$$

The polynomial $\hat{F}(p)$ will be said to have weight w, if w is the degree of the polynomial $F(x)$; it will be said to be w-homogeneous if $F(x)$ is.

The elements of a (minimal) basis of $\mathbb{R}[x]^G$ can be chosen to be homogeneous polynomials. The number q of elements of a minimal integrity basis and their homogeneity *degrees* d_i's are only determined by the group G.

To avoid trivial situations, in this paper we shall only consider linear groups with no fixed points, but for the origin of $\mathbb{R}^n$. In this case, the minimum degree of the elements of a minimal integrity basis is necessarily 2, and the following conventions can be adopted:

$$d_1 \geqslant d_2 \geqslant \ldots d_q = 2 \qquad p_q(x) = \|x\|^2 = \sum_1^n {}_i x_i^2\,. \tag{8}$$

Hereafter, by a minimal integrity basis of G (abbreviated into MIB of G) we shall always mean a *minimal homogeneous integrity basis* for the ring of G-invariant polynomials, for which the conventions of (8) hold true.

Since G is a compact group, the orbits of G are separated by the elements of a MIB of G, i.e. at least one element of a MIB of G takes on different values on two distinct orbits. Thus, the elements of a MIB of G provide a good parametrization of the points of $\mathbb{R}^n/G$, that turns out to also be smooth, since the orbit map $p : \mathbb{R}^n \longrightarrow \mathbb{R}^q$, which maps all the points of $\mathbb{R}^n$ lying on an orbit of G onto a single point of $\mathbb{R}^q$, induces a diffeomorphism of $\mathbb{R}^n/G$ onto a semialgebraic q-dimensional connected closed subset of $\mathbb{R}^q$.

2.3. *Coregular and non-coregular groups*

The group G is said to be *coregular* if the elements of its MIBs are algebraically, and therefore functionally, independent. If G is non-coregular, the elements of any one of its MIBs satisfy a certain number of algebraic identities in $\mathbb{R}^n$:

$$\hat{F}_A(p(x)) = 0 \qquad A = 1, \ldots, K\,. \tag{9}$$

The associated equations

$$\hat{F}_A(p) = 0 \qquad A = 1, \ldots, K \tag{10}$$

define an algebraic variety in $\mathbb{R}^q$, which will be called the *variety $\mathcal{Z}$ of the relations* (among the elements of the MIB). The number K will be said the *coregularity order* of G. If G is coregular, there are no relations among the elements of its MIBs, the coregularity order of G is zero and we shall set $\mathcal{Z} = \mathbb{R}^n$.

From now on, in this paper, we shall deal with coregular CLGs.

2.4. The $\hat{P}(p)$ matrix

A characterization of the image $p(\mathbb{R}^n)$ of the orbit space of G as a semi-algebraic variety can be easily obtained through a matrix $\hat{P}(p)$, defined only in terms of the G-invariant Euclidean scalar products between the gradients of the elements of the MIB $\{p(x)\}$:

$$P_{ab}(x) = \sum_1^n {}_i \frac{\partial p_a(x)}{\partial x_i}\frac{\partial p_b(x)}{\partial x_i} = \hat{P}_{ab}(p(x)) \qquad a, b = 1, \ldots, q \tag{11}$$

where in the last member, use has been made of Hilbert's theorem, in order to express $P_{ab}(x)$ as a polynomial function of $p_1(x), \ldots, p_q(x)$.

The following fundamental theorem clarifies the meaning and points out the role of the matrix $\hat{P}(p)$:

Theorem 2.1. Let G be a compact coregular subgroup of $O_n(\mathbb{R})$, p the map $\mathbb{R}^n \to \mathbb{R}^q$ defined by the homogeneous MIB $\{p_1(x), p_2(x), \ldots, p_q(x)\}$ and $\hat{P}(p)$ the matrix defined in (11). Then $\bar{\mathcal{S}} = p(\mathbb{R}^n)$ is the unique semialgebraic connected subset of the variety $\mathcal{Z} \subseteq \mathbb{R}^q$ of the relations among the elements of the MIB where $\hat{P}(p)$ is positive semi-definite. The k-dimensional primary strata of $\bar{\mathcal{S}}$ are the connected components of the set $\hat{W}^{(k)} = \{p \in \mathcal{Z}; |\ \hat{P}(p) \geqslant 0, \mathrm{rank}(\hat{P}(p)) = k\}$; they are the images of the connected components of the k–dimensional isotropy type strata of $\mathbb{R}^n/G$. In particular, the variety $\mathcal{S}$ of the interior points of $\bar{\mathcal{S}}$, where $\hat{P}(p)$ has the maximum rank, is the image of the principal stratum.

It will be worthwhile to note that, for coregular groups, $\mathcal{Z} = \mathbb{R}^q$ and that the image of the unit sphere of $\mathbb{R}^n$ under the orbit map $p(x)$ is a *compact connected* $(q-1)$-dimensional semialgebraic variety in the space $\mathbb{R}^{q-1}$ spanned by the variables $p_1, \ldots, p_{q-1}$.

The following properties, which are common to all the matrices $\hat{P}(p)$, are more or less immediate consequences of the definition of these matrices:

P1 *Symmetry, homogeneity and bounds on the last row and column.* The matrix $\hat{P}(p)$ is a $q \times q$ symmetric matrix, whose elements $\hat{P}_{ab}(p)$ are real w-homogeneous polynomials with weight

$$w(\hat{P}_{ab}) = d_a + d_b - 2\,. \tag{12}$$

The last row and column are determined by the degrees of the MIB:

$$\hat{P}_{qa}(p) = \hat{P}_{aq}(p) = 2d_a p_a \qquad a = 1, 2, \ldots, q\,. \tag{13}$$

P2 *Tensor character.* The matrix elements of $\hat{P}(p)$ transform as the components of a rank 2 contravariant tensor under MIB transformations that maintain the conventions fixed in (8) (these transformations will be hereafter called MIBTs). In fact, let $\{p(x)\}$ and $\{p'(x)\}$ be distinct MIBs; the $p'_a(x)$'s, being G-invariant polynomials, can be expressed as polynomial functions of the $p_a(x)$'s:

$$p'_\alpha = p'_\alpha(p) \qquad \alpha = 1, 2, \ldots, q-1 \tag{14}$$

where the polynomial function $p'_\alpha(p)$ only depends on the p_a's such that† $d_a \leqslant d'_\alpha$. Then,

$$\hat{P}'(p'(p)) = J(p)\hat{P}(p)J^T(p) \tag{15}$$

where we have denoted by $J(p)$ the Jacobian matrix of the transformation:

$$J_{ab}(p) = \partial p'_a(p)/\partial p_b \qquad a, b = 1, \ldots, q \tag{16}$$

† Since in our conventions the qth element of any MIB is fixed to equal $\sum_{1_i}^n x_i^2$, when defining a MIBT we shall always understand the condition $p'_q(p) = p_q$.

the matrix J turns out to be upper-block triangular and the determinant of $\hat{P}(p)$ to be a relative invariant of the group of the MIBTs.

2.5. Classification of the orbit spaces of CCLGs

Two matrices $\hat{P}(p)$ and $\hat{P}'(p')$ will be said to be *equivalent* if they are connected by a relation like (15), where $J(p)$ is the Jacobian matrix of a MIBT $p' = p'(p)$. Thus, the $\hat{P}$-matrices computed from different MIBs of the same CLG are equivalent, and the semialgebraic varieties $\bar{\mathcal{S}}$ and $\bar{\mathcal{S}}'$ defined by the positivity conditions imposed on $\hat{P}(p)$ and $\hat{P}'(p')$, respectively, are equivalent concrete realizations of the orbit space $\mathbb{R}^n/G$.

Since G is coregular, its orbit space is completely determined by the positivity conditions of a $\hat{P}$-matrix computed from any one of its MIBs; for non-coregular groups, also a complete set of relations among the p_a's has to be specified.

2.6. Isomorphism classes of orbit spaces

The notions of MIBTs (see equation (14)) and of equivalence of $\hat{P}$-matrices (see equation (15)) can be extended to the case of different coregular groups G and G', provided that their MIBs have the same number of elements, with the same degrees. Let, $\{p\}$ and $\{p'\}$ be MIBs for G and G', respectively.

Definition 2.1. The orbit space $\mathbb{R}^n/G$ and $\mathbb{R}^{n'}/G'$ of the compact coregular linear groups G and G' will be said to be isomorphic if the associated $\hat{P}$-matrices $\hat{P}(p)$ and $\hat{P}'(p')$ satisfy (15), where the transformation $p' = p'(p)$ has all the formal properties of a MIBT.

If G and G' have isomorphic orbit spaces, then the images of their orbit spaces $\bar{\mathcal{S}}$ and $\bar{\mathcal{S}}'$, associated with the MIBs $\{p\}$ and $\{p'\}$ are isomorphic semialgebraic varieties:

$$\bar{\mathcal{S}}' = p'(\bar{\mathcal{S}})\,. \tag{17}$$

Thus the classification of the isomorphism classes of the orbit spaces of the CCLGs rests on the determination of a representative for each class of equivalent $\hat{P}(p)$ matrices (and, for non-coregular groups, on the determination of the possible relations among the elements of the MIBs). This can be done, in principle, for all CCLGs. The matrices $\hat{P}(p)$ have been shown [36], in fact, to be solutions of a *canonical differential equation*, satisfying convenient initial conditions (*allowable* solutions). The canonical equation does involve only the degrees $\{d_1, d_2, \dots, d_q\}$ of the MIBs as free parameters, as we shall see in the next subsection.

2.7. Boundary and positivity conditions

For coregular groups, the orbit space $\bar{\mathcal{S}}$, defined in theorem 2.1, is a connected q-dimensional semialgebraic variety of $\mathbb{R}^q$ and, like all semialgebraic varieties [47], it presents a natural stratification in connected semialgebraic sub-varieties $\hat{\sigma}$, called *primary strata*† We shall denote by $\mathcal{I}(\hat{\sigma})$ the ideal formed by all the polynomials in $p \in \mathbb{R}^q$ vanishing on $\hat{\sigma}$. Every $\hat{f}(p) \in \mathcal{I}(\hat{\sigma})$ defines an invariant polynomial function in $\mathbb{R}^n$ vanishing at all the points x lying in the set $\Sigma_f = p^{-1}(\hat{\sigma})$:

$$f(x) = \hat{f}(p(x)) = 0 \qquad \forall x \in \Sigma_f\,. \tag{18}$$

† A simple example of a compact connected semialgebraic variety of $\mathbb{R}^3$ is yielded by a polyhedron. Its interior points form its unique three-dimensional primary stratum, while two-, one- and zero-dimensional primary strata are formed, respectively, by the interior points of each face, by the interior points of each edge, by each vertex.

The gradient $\partial f(x)$ is obviously orthogonal to Σ_f at every $x \in \Sigma_f$, but, it must also be tangent to Σ_f since $f(x)$ is a G-invariant function [43, 24]. As a consequence,

$$0 = \partial f(x) = \sum_1^q {}_b \partial_b \hat{f}(p)\Big|_{p=p(x)} \partial p_b(x) \qquad \forall x \in \Sigma_f \,. \tag{19}$$

By taking the scalar product of (19) with $\partial p_a(x)$, we end up with the following *boundary conditions* [38]:

$$\sum_1^q {}_b \hat{P}_{ab}(p)\partial_b \hat{f}(p) \in \mathcal{I}(\hat{\sigma}) \qquad \forall \hat{f} \in \mathcal{I}(\hat{\sigma}) \qquad \text{and} \qquad \forall \hat{\sigma} \subseteq \bar{\mathcal{S}} \,. \tag{20}$$

If $\{Q_1^{(\hat{\sigma})}(p), Q_2^{(\hat{\sigma})}(p), \ldots, Q_m^{(\hat{\sigma})}(p)\}$ is an integrity basis for $\mathcal{I}(\hat{\sigma})$, (20) is equivalent to

$$\sum_1^q {}_b \hat{P}_{ab}(p)\partial_b Q_r^{(\hat{\sigma})}(p) = \sum_1^m {}_s \lambda_{rs;a}^{(\hat{\sigma})}(p)\, Q_s^{(\hat{\sigma})} \tag{21}$$

where the λ's are w-homogeneous polynomial functions of p.

In the particular case in which $\hat{\sigma}$ is a $(q-1)$-dimensional primary stratum, the ideal $\mathcal{I}(\hat{\sigma})$ has a unique *irreducible* generator, $Q^{(\hat{\sigma})}(p)$, and (21) reduces to the simpler form [36, 38]

$$\sum_1^q {}_b \hat{P}_{ab}(p)\partial_b Q^{(\hat{\sigma})}(p) = \lambda_a^{(\hat{\sigma})}(p)\, Q^{(\hat{\sigma})}(p) \qquad a = 1, \ldots, q \,. \tag{22}$$

The validity of (21) can be extended to the case in which $\hat{\sigma}$ is a union of primary strata. In particular, the ideal $\mathcal{I}(\mathcal{B})$, associated to the union $\mathcal{B}$ of all the $(q-1)$-dimensional strata of $\bar{\mathcal{S}}$ (whose closure forms the boundary of $\bar{\mathcal{S}}$) has a unique generator $A(p)$:

$$A(p) = \prod_{\hat{\sigma} \subseteq \mathcal{B}} Q^{(\hat{\sigma})}(p) \tag{23}$$

and the following relation is satisfied:

$$\sum_1^q {}_b \hat{P}_{ab}(p)\, \partial_b A(p) = \lambda_a^{(A)}(p) A(p) \tag{24}$$

where $\lambda^{(A)}(p)$ is a contravariant vector field with w-homogeneous components, and

$$\lambda^{(A)}(p) = \sum_{\hat{\sigma} \subseteq \mathcal{B}} \lambda^{(\hat{\sigma})}(p) \,. \tag{25}$$

The results summarized below have been proved in [37].

The vector $\lambda^{(A)}(p)$ can be reduced to the canonical form $\lambda_a^{(A)}(p) = 2\delta_{aq} w(A)$ in particular MIBs, the so-called *A-bases*, which are intrinsically defined. In an A-basis, the boundary conditions assume the following *canonical* form:

$$\sum_1^q {}_b \hat{P}_{ab}(p)\partial_b A(p) = 2\delta_{aq} w(A) A(p) \qquad a = 1, \ldots, q \,. \tag{26}$$

From equation (26) one deduces that, in every A-basis, the following facts hold true:

(i) The point $p^{(0)} = (0, \ldots, 0, 1)$ lies in $\mathcal{S}$; it is the image of a G-orbit lying on the unit sphere of $\mathbb{R}^n$.

(ii) $A(p)$ is a factor of det $\hat{P}(p)$; its weight is bounded:

$$2d_1 \leqslant w(A) \leqslant w(\det \hat{P}) = 2\sum_{1}^{q}{}_{a} d_a - 2q \tag{27}$$

and it can be normalized at $p^{(0)}$:

$$A(p^{(0)}) = 1 \tag{28}$$

we shall call it the *complete active factor* of det $\hat{P}(p)$.

(iii) The restriction, $A(p)|_{p_q=1}$, of $A(p)$ to the image of the unit sphere of $\mathbb{R}^n$ in $\mathbb{R}^q$ has a unique local non-degenerate maximum lying at $p^{(0)}$; thus,

$$\partial_\alpha A(p)|_{p=p^{(0)}} = 0 \qquad \alpha = 1, \ldots, q-1\,. \tag{29}$$

(iv) $\hat{P}(p^{(0)})$ is block diagonal, each block being associated to a subset of p_a's sharing the same degree, and, in a subclass of A-bases (*standard A-bases*), it is diagonal:

$$\hat{P}_{ab}(p^{(0)}) = d_a d_b \delta_{ab} \qquad a, b = 1, \ldots, q\,. \tag{30}$$

Two different standard A-bases are related by a MIBT not involving p_q:

$$p'_\alpha = f_\alpha(p_1, \ldots, p_{q-1}) \qquad \alpha = 1, \ldots, q-1 \tag{31}$$

the corresponding Jacobian matrix is orthogonal at $p^{(0)}$.

2.8. *The canonical equation*

Let us now look at the boundary conditions from a different point of view: the set $\{p_1, \ldots, p_q\}$ will be viewed as a set of *weighted indeterminates*, with integer weights $d_1, \ldots, d_q$ satisfying the conventions

$$d_1 \geqslant d_2 \geqslant \ldots d_q = 2 \tag{32}$$

and the boundary conditions expressed in (26) will be considered as a set of equations in which $\hat{P}_{ab}(p)$ and $A(p)$ are thought of as unknown polynomial functions of p, satisfying the conditions listed under items P1, P2 and in (27). The positivity conditions specified in (28) and (30) will be treated as initial conditions. With the above meaning for the symbols, (26) will be called the *canonical equation*.

The solutions $(\hat{P}(p), A(p))$ of the canonical equation satisfying the initial conditions specified in (28) and (30) will be called *allowable solutions* and the corresponding $\hat{P}$ matrices, *allowable $\hat{P}$ matrices*.

A solution of the canonical equation will be said to be *irreducible*, if $A(p)$ is an irreducible (real) polynomial and *fully active*, if $A(p) = \text{constant} \times \det \hat{P}(p)$.

Two allowable $\hat{P}$ matrices will be said to be equivalent if a w-homogeneous transformation exists on the indeterminates $p_1, \ldots, p_{q-1}$ such that (15) is satisfied.

The allowable $\hat{P}$-matrices $\hat{P}(p)|_{p_q=1}$ have been shown to be positive semi-definite only in a compact $(q-1)$-dimensional semialgebraic variety of the space $\mathbb{R}^{q-1}$ spanned by the variables $p_1, \ldots, p_{q-1}$, containing the point $p^{(0)}$.

All the $\hat{P}$-matrices associated to the different MIBs of any CCLG with no fixed points are necessarily equivalent to an allowable $\hat{P}$-matrix. At present we do not know if the converse holds also true, i.e. if every *allowable* $\hat{P}$-matrix is generated by a CCLG with no fixed points.

The allowable solutions of the canonical equations for $q \leqslant 4$ have been determined in I and II. For each choice of the degrees $\{d_1, d_2, \ldots, d_q\}$, only a finite or null number of non-equivalent solutions has been found, showing the existence of *selection rules* for the degrees of the CCLGs. The solutions can be organized in *towers*; the degrees of the elements of the same tower can be written in the form $d_\alpha = s d_\alpha^{(0)}$, $\alpha = 1, \dots, q-1$, where s is an integer scale parameter. A solution of the canonical equation corresponding to $s = 1$ will be said a *fundamental* solution.

Exploiting the fact that all the *finite* coregular linear groups have been classified in the mathematical literature and the associated MIBs have been determined [48], in the following sections we shall determine the $\hat{P}$-matrices of all the finite CLGs with two-, three- [38] and four-dimensional [39] orbit spaces, and we shall check that they can all be found among the allowable solutions of the canonical equation listed in I and II.

3. Irreducible reflection groups with 2, 3 and 4 basic invariants

Finite groups generated by reflections exhaust the class of *finite* CLGs. The explicit form of the elements of at least one MIB is known for all these groups [27–32]. Thus, the corresponding $\hat{P}(p)$ matrices can be computed, as well as the complete factors $A(p)$ of det $\hat{P}(p)$ and the vector fields $\lambda^{(A)}(p)$ appearing in (24).

In general, the MIBs proposed in the literature do not correspond to A-bases, so the comparison with the results reported in I and II is not immediate. The easiest way to determine the form of a MIBT leading to an A-basis is through the following condition on the Jacobian matrix $J_{ab}(p)$ of the transformation:

$$\lambda'^{(A)}_a(p'(p)) = \sum_1^q {}_b J_{ab}(p)\, \lambda_b^{(A)}(p) = 0 \qquad a = 1, 2, \dots, (q-1)\,. \tag{33}$$

When the A-basis is not unique, (33) is not sufficient to determine all the free parameters involved in the definition of the MIBT. The residual free parameters can, however, be determined by requiring that the parametric expression of $\hat{P}'(p')$ in a general A-basis coincides with an allowable $\hat{P}$-matrix listed in I or II. To shorten our formulae and to make easier the comparison, we shall define

$$\tilde{p} = (p_1, \dots, p_{q-1}, 1) \qquad \text{for} \quad p = (p_1, \dots, p_q) \tag{34}$$

$$\check{x} = (x_1, \dots, x_n, 0) \qquad \text{for} \quad x = (x_1, \dots, x_n) \tag{35}$$

$$R_{ab} = \hat{P}_{ab}/d_a d_b \qquad a, b = 1, \dots, q \tag{36}$$

$$f_{n,k}(x) = \sum_1^n {}_i x_i^{n+1-k} \qquad \text{for} \quad x = (x_1, \dots, x_n)\,. \tag{37}$$

3.1. Irreducible CCLGs with two basic invariants

The irreducible CCLGs with two-dimensional orbit spaces are classified in the mathematical literature according to the following *types*: A_2, B_2, G_2 and $I_2(m)$. The type G_2 and $I_2(6)$ groups have the same invariants, so we shall not discuss separately the group of type G_2.

3.2. Type A_2

The group acts on the plane $y_1 + y_2 + y_3 = 0$ of $\mathbb{R}^3$ by permutations. Therefore the group and its invariants can be obtained from the reduction of the group S_3, acting on $y = (y_1, y_2, y_3)$ by permutations of the coordinates.

A MIB for S_3 is yielded by $\{f_{3,1}(y), f_{3,2}(y), f_{3,3}(y)\}$, where $f_{3,k}$ is defined in (37). The reduction of the linear group S_3 can be obtained by means of an orthogonal basis transformation in $\mathbb{R}^3$, induced by the matrix

$$A = \frac{1}{6}\begin{pmatrix} \sqrt{3} & -\sqrt{3} & 0 \\ 1 & 1 & -2 \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{pmatrix}. \tag{38}$$

The elements of the linear group of type A_2 are obtained as the principal minors built with the first two rows and columns of the matrices AgA^{-1}, $g \in S_3$ and, after setting, for $x = (x_1, \ldots, x_n)$,

$$p_a(x) = \tilde{p}_a(A^{-1}\check{x}) \tag{39}$$

and $x = (x_1, x_2)$, a MIB for A_2 is yielded by $\{p_1(x), p_2(x)\}$ or, explicitly,

$$p_1(x) = x_2\left(3x_1^2 - x_2^2\right)/\sqrt{6} \qquad p_2(x) = x_1^2 + x_2^2 \,. \tag{40}$$

The unique element of the associated reduced $\hat{P}$-matrix is easily calculated to be

$$\hat{P}_{11}(p) = 3p_2^2/2 \tag{41}$$

and after the following MIBT:

$$p_1' = \sqrt{6}\, p_1 \tag{42}$$

one obtains, for $p_2' = 1$, the allowable $\hat{P}(p)$ matrix determined in I for $q = 2$ and $d_1 = 3$:

$$R_{11}'(\tilde{p}') = 1 \,. \tag{43}$$

3.3. Type B_2

The group acts on $x = (x_1, x_2)$ by permutations and sign changes of the coordinates. A MIB can be chosen as follows:

$$p_1(x) = x_1^4 + x_2^4 \qquad p_2(x) = x_1^2 + x_2^2 \,. \tag{44}$$

The unique essential element of the associated $\hat{P}$-matrix turns out to be the following:

$$\hat{P}_{11}(p) = 8p_2\big(3p_1 - p_2^2\big) \tag{45}$$

and after the following MIBT:

$$p_1' = 4p_1 - 3p_2^2 \tag{46}$$

one obtains, for $p_2' = 1$, the allowable $\hat{R}(p)$ matrix determined in I for $q = 2$ and $d_1 = 4$:

$$R_{11}'(\tilde{p}') = 1 \,. \tag{47}$$

3.4. *Type* $I_2(m)$, $m \geqslant 3$

The groups of type $I_2(m)$, $m \geqslant 3$, are the dihedral groups $\mathcal{D}_m$, defined as the groups of orthogonal transformations of $\mathbb{R}^2$ which preserve a regular m-sided polygon centred at the origin. After setting

$$z = x_1 + \mathrm{i}x_2 \tag{48}$$

a MIB of $\mathcal{D}_m$ is yielded, for instance, by the invariants $p(x) = \{p_1(x), p_2(x)\}$, with

$$p_1(x) = \Re z^m \qquad p_2(x) = |z|^2 = x_1^2 + x_2^2\,. \tag{49}$$

The unique essential element of the associated $\hat{P}$-matrix turns out to be the following:

$$\hat{P}_{11}(p) = d_1^2\, p_2^{m-1}\,. \tag{50}$$

A comparison with I shows that $\{p\}$ is a standard A-basis.

3.5. *Type* A_3

The group acts on the plane $y_1 + y_2 + y_3 + y_4 = 0$ of $\mathbb{R}^4$ by permutations. Therefore the group and its invariants can be obtained from the reduction of the group S_4, acting on $y = (y_1, y_2, y_3, y_4)$ by permutations of the coordinates.

A MIB for S_4 is yielded by $\{f_1(y), \ldots, f_4(y)\}$, where f_k is defined in (37). The reduction of the linear group S_4 can be obtained by means of an orthogonal basis transformation in $\mathbb{R}^4$, induced by the matrix

$$A = \frac{1}{6}\begin{pmatrix} 3\sqrt{2} & -3\sqrt{2} & 0 & 0 \\ \sqrt{6} & \sqrt{6} & -2\sqrt{6} & 0 \\ \sqrt{3} & \sqrt{3} & \sqrt{3} & -3\sqrt{3} \\ 3 & 3 & 3 & 3 \end{pmatrix}. \tag{51}$$

The elements of the group of type A_3 are obtained as the principal minors built with the first three rows and columns of the matrices AgA^{-1}, $g \in S_4$ and, after setting $x = (x_1, x_2, x_3)$, a MIB is yielded by $\{p_1(x), p_2(x), p_3(x)\}$, with $p_a(x)$ defined in (39); explicitly:

$$\begin{aligned} p_1(x) &= \big(6x_1^4 + 12x_1^2x_2^2 + 6x_2^4 + 12\sqrt{2}\,x_1^2x_2x_3 - 4\sqrt{2}\,x_2^3x_3 + 6x_1^2x_3^2 + 6x_2^2x_3^2 + 7x_3^4\big)/12 \\ p_2(x) &= \big(3\sqrt{2}\,x_1^2x_2 - \sqrt{2}\,x_2^3 + 3x_1^2x_3 + 3x_2^2x_3 - 2x_3^3\big)/2\sqrt{3} \\ p_3(x) &= x_1^2 + x_2^2 + x_3^2\,. \end{aligned} \tag{52}$$

The essential elements of the associated $\hat{P}(p)$-matrix turn out to be the following:

$$\begin{aligned} \hat{P}_{11}(p) &= 2\big(18p_1p_3 + 2p_2^2 - 3p_3^3\big)/3 \\ \hat{P}_{12}(p) &= 7p_2p_3 \\ \hat{P}_{22}(p) &= 9\big(4p_1 - p_3^2\big)/4 \end{aligned} \tag{53}$$

and after the following MIBT:

$$p_1' = 12p_1 - 5p_3^2 \qquad p_2' = 2\sqrt{3}p_2 \tag{54}$$

one obtains, for $p_3' = 1$, the matrix R of class III.1 ($m = 1$), reported in I:

$$\begin{aligned} R_{11}'(\tilde{p}') &= -{p'}_1 + {p_2'}^2 + 2 \\ R_{12}'(\tilde{p}') &= 2{p'}_2 \\ R_{22}'(\tilde{p}') &= p_1' + 2\,. \end{aligned} \tag{55}$$

3.6. Type B_3

The group acts on $x = (x_1, x_2, x_3)$ by permutations and sign changes of the coordinates. A MIB can be chosen as follows:

$$p_1(x) = x_1^6 + x_2^6 + x_3^6 \qquad p_2(x) = x_1^4 + x_2^4 + x_3^4 \qquad p_3(x) = x_1^2 + x_2^2 + x_3^2 \,. \tag{56}$$

The essential elements of the associated $\hat{P}(p)$-matrix turn out to be the following:

$$\begin{aligned} \hat{P}_{11}(p) &= 30p_1p_2 + 30p_1p_3^2 - 30p_2p_3^3 + 6p_3^5 \\ \hat{P}_{12}(p) &= 32p_1p_3 + 12p_2^2 - 24p_2p_3^2 + 4p_3^4 \\ \hat{P}_{22}(p) &= 16p_1 . \end{aligned} \tag{57}$$

and after the following MIBT:

$$p_1' = 324p_1 - 432p_2p_3 + 124p_3^3 \qquad p_2' = 18p_2 - 10p_3^2 \tag{58}$$

one obtains, for $p_3' = 1$, the matrix R of class III.2 ($m = 1$) reported in I:

$$\begin{aligned} R'_{11}(\tilde{p}') &= -p_1'p_2' - 4p_1' + 8{p_2'}^2 - 16p_2' + 64 \\ R'_{12}(\tilde{p}') &= -2p_1' + {p_2'}^2 + 12p_2' \\ R'_{22}(\tilde{p}') &= p_1' + 4p_2' + 16 \,. \end{aligned} \tag{59}$$

3.7. Type D_3

The group acts on $x = (x_1, x_2, x_3)$ by permutations and by changes of an even number of signs of the coordinates. A MIB can be chosen as follows:

$$p_1 = x_1^4 + x_2^4 + x_3^4 \qquad p_2 = x_1x_2x_3 \qquad p_3 = x_1^2 + x_2^2 + x_3^2 \,. \tag{60}$$

The essential elements of the associated $\hat{P}$-matrix turn out to be the following:

$$\begin{aligned} \hat{P}_{11}(p) &= 24p_1p_3 + 48p_2^2 - 8p_3^3 \\ \hat{P}_{12}(p) &= 4p_2p_3 \\ \hat{P}_{22}(p) &= (-p_1 + p_3^2)/2 \end{aligned} \tag{61}$$

and, after the following MIB transformation:

$$p_1' = 4p_3^2 - 6p_1 \qquad p_2' = 6\sqrt{3}p_2 \tag{62}$$

one obtains, for $p_3' = 1$, the matrix R of class III.1 ($m = 1$) reported in I. The orbit spaces of the linear groups A_3 and D_3 turn out to be isomorphic.

3.8. Type H_3

The group is the symmetry group of the icosahedron in $\mathbb{R}^3$.

Let us denote by τ the golden ratio:

$$\tau = (1 + \sqrt{5})/2 \,. \tag{63}$$

Then, according to [31], a MIB for the group can be chosen as follows:

$$\begin{aligned}
p_1(x) &= (1+\tau^2)^{-5}\left[(1+\tau^{10})(x_1^{10}+x_2^{10}+x_3^{10})+45\tau^2(x_1^2x_2^8+x_2^2x_3^8+x_3^2x_1^8)\right.\\
&\quad +210\tau^4(x_1^4x_2^6+x_2^4x_3^6+x_3^4x_1^6)+210\tau^6(x_1^6x_2^4+x_2^6x_3^4+x_3^6x_1^4)\\
&\quad \left.+45\tau^8(x_1^8x_2^2+x_2^8x_3^2+x_3^8x_1^2)\right]\\
p_2(x) &= (1+\tau^2)^{-3}\left[(1+\tau^6)(x_1^6+x_2^6+x_3^6)+15\tau^2(x_1^2x_2^4+x_2^2x_3^4+x_1^4x_3^2)\right.\\
&\quad \left.+\,15\tau^4(x_1^4x_2^2+x_2^4x_3^2++x_1^2x_3^4)\right]\\
p_3(x) &= x_1^2+x_2^2+x_3^2\,.
\end{aligned} \tag{64}$$

The essential elements of the associated $\hat{P}$-matrix turn out to be the following:

$$\begin{aligned}
\hat{P}_{11}(p) &= 192p_1p_2p_3+336p_1p_3^4/5+16p_2^3/9-1136p_2^2p_3^3/15-15\,968p_2p_3^6/75\\
&\quad +81\,412p_3^9/1125\\
\hat{P}_{12}(p) &= 336p_1p_3^2/5+184p_2^2p_3/3-404p_2p_3^4/3+2656p_3^7/75\\
\hat{P}_{22}(p) &= 18p_1-12p_2p_3^2+174p_3^5/25
\end{aligned} \tag{65}$$

and, after the following MIBT:

$$p_1' = (50\,625p_1-123\,750p_2p_3^2+39\,285p_3^5)/2 \qquad p_2' = 225p_2-93p_3^3 \tag{66}$$

one obtains, for $p_3'=1$, the matrix R of class III.3($m=1$) reported in I:

$$\begin{aligned}
R'_{11}(\tilde{p}') &= 1152-12p_1'-168p_2'-4p_1'p_2'+44{p_2'}^2+{p_2'}^3\\
R'_{12}(\tilde{p}') &= -6p_1'+60p_2'+5{p_2'}^2\\
R'_{22}(\tilde{p}') &= 96+p_1'+14p_2'\,.
\end{aligned} \tag{67}$$

3.9. *Type A_4*

The group acts on the plane $y_1+y_2+y_3+y_4+y_5=0$ of $\mathbb{R}^5$ by permutations. Therefore the group and its invariants can be obtained from the reduction of the group S_5, acting on $y=(y_1,\ldots,y_5)$ by permutations of the coordinates.

A MIB for S_5 is yielded by $\{f_{5,1}(y),\ldots,f_{5,5}(y)\}$, where $f_{5,k}$ is defined in (37). The reduction of the linear group S_5 can be obtained by means of an orthogonal basis transformation in $\mathbb{R}^5$, induced by the matrix

$$A = \begin{pmatrix}
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0\\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & 0 & 0\\
\frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{3}{2\sqrt{3}} & 0\\
\frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} & -\frac{4}{2\sqrt{5}}\\
\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}}
\end{pmatrix}. \tag{68}$$

The elements of the group of type A_4 are obtained as the principal minors built with the first four rows and columns of the matrices AgA^{-1}, $g\in S_5$ and, after setting $x=(x_1,\ldots,x_4)$, a MIB is yielded by $\{p_1(x), \ldots p_4(x)\}$, where $p_a(x)$ is defined in (39); explicitly,

$$\begin{aligned}
p_1(x) = 1800^{-1}\big(&750\sqrt{6}x_1^4x_2 + 500\sqrt{6}x_1^2x_2^3 - 250\sqrt{6}\,x_2^5 + 750\sqrt{3}\,x_1^4x_3 + 1500\sqrt{3}\,x_1^2x_2^2x_3 \\
&+750\sqrt{3}\,x_2^4x_3 + 750\sqrt{6}\,x_1^2x_2x_3^2 - 250\sqrt{6}\,x_2^3x_3^2 + 250\sqrt{3}\,x_1^2x_3^3 + 250\sqrt{3}\,x_2^2x_3^3 \\
&-500\sqrt{3}\,x_3^5 + 450\sqrt{5}\,x_1^4x_4 + 900\sqrt{5}\,x_1^2x_2^2x_4 + 450\sqrt{5}\,x_2^4x_4 \\
&+900\sqrt{10}\,x_1^2x_2x_3x_4 - 300\sqrt{10}\,x_2^3x_3x_4 + 450\sqrt{5}\,x_1^2x_3^2x_4 + 450\sqrt{5}\,x_2^2x_3^2x_4 \\
&+525\sqrt{5}\,x_3^4x_4 + 450\sqrt{6}\,x_1^2x_2x_4^2 - 150\sqrt{6}\,x_2^3x_4^2 + 450\sqrt{3}\,x_1^2x_3x_4^2 \\
&+450\sqrt{3}\,x_2^2x_3x_4^2 - 300\sqrt{3}\,x_3^3x_4^2 + 90\sqrt{5}\,x_1^2x_4^3 + 90\sqrt{5}\,x_2^2x_4^3 90\sqrt{5}\,x_3^2x_4^3 \\
&-459\sqrt{5}\,x_4^5\big) \qquad (69)\\
p_2(x) = 60^{-1}\big(&30x_1^4 + 60x_1^2x_2^2 + 30x_2^4 + 60\sqrt{2}\,x_1^2x_2x_3 - 20\sqrt{2}\,x_2^3x_3 + 30x_1^2x_3^2 + 30x_2^2x_3^2 \\
&+35x_3^4 + 12\sqrt{30}\,x_1^2x_2x_4 - 4\sqrt{30}\,x_2^3x_4 + 121\sqrt{5}\,x_1^2x_3x_4 + 121\sqrt{5}\,x_2^2x_3x_4 \\
&-81\sqrt{5}\,x_3^3x_4 + +18x_1^2x_4^2 + 18x_2^2x_4^2 + 18x_3^2x_4^2 + 39x_4^4\big) \\
p_3(x) = 30^{-1}\big(&15\sqrt{6}\,x_1^2x_2 - 5\sqrt{6}\,x_2^3 + 15\sqrt{3}\,x_1^2x_3 + 15\sqrt{3}\,x_2^2x_3 - 10\sqrt{3}\,x_3^3 + 9\sqrt{5}\,x_1^2x_4 \\
&+9\sqrt{5}\,x_2^2x_4 + 9\sqrt{5}\,x_3^2x_4 - 9\sqrt{5}\,x_4^3\big) \\
p_4(x) = x_1^2 &+ x_2^2 + x_3^2 + x_4^2\,.
\end{aligned}$$

The essential elements of the associated $\hat{P}(p)$-matrix turn out to be the following:

$$\begin{aligned}
\hat{P}_{11}(p) &= 5\left(12p_2^2 + 128p_1p_3 + 20p_2p_4^2 - 5p_4^4\right)/48 \\
\hat{P}_{12}(p) &= \left(46p_2p_3 + 84p_1p_4 - 35p_3p_4^2\right)/6 \\
\hat{P}_{13}(p) &= \left(40p_3^2 + 66p_2p_4 - 15p_4^3\right)/8 \\
\hat{P}_{22}(p) &= 2\left(16p_3^2 + 90p_2p_4 - 15p_4^3\right)/15 \\
\hat{P}_{23}(p) &= 12\,(5p_1 - p_3p_4)\,/5 \\
\hat{P}_{33}(p) &= 9\left(5p_2 - p_4^2\right)/5
\end{aligned} \qquad (70)$$

and, after the following MIBT:

$$p'_1 = 30\sqrt{15}\,(4p_1 - 3p_3p_4) \qquad p'_2 = 3\left(20p_2 - 7p_4^2\right) \qquad p'_3 = 6\sqrt{15}p_3 \qquad (71)$$

one obtains, for $p'_3 = 1$, the matrix R of class $E_1(s = 1)$, reported in II:

$$\begin{aligned}
R'_{11}(\tilde{p}') &= -4p'_1p'_3 + 3{p'_2}^2 - 27p'_2 + 18(2{p'_3}^2 + 9) \\
R'_{12}(\tilde{p}') &= -6p'_1 + p'_3(5p'_2 + 54) \\
R'_{13}(\tilde{p}') &= 2(3p'_2 + {p'_3}^2) \\
R'_{22}(\tilde{p}') &= 3p'x_2 + 2(4{p'_3}^2 + 27) \\
R'_{23}(\tilde{p}') &= p'_1 + 12p'_3 \\
R'_{33}(\tilde{p}') &= p'_2 + 9\,.
\end{aligned} \qquad (72)$$

3.10. Type B_4

The group acts on $x = (x_1, x_2, x_3, x_4)$ by permutations and sign changes of the coordinates. A MIB can be chosen as follows:

$$\left\{p_a(x) = \sum_1^4{}_i\, x_i^{10-2a}\right\}_{1\leqslant a\leqslant 4}. \qquad (73)$$

In this basis the essential elements of the $\hat{P}(p)$ matrix turn out to be the following:

$$\begin{aligned}
\hat{P}_{11}(p) &= 4\left(28p_1p_2 + 14p_2p_3^2 + 42p_1p_3p_4 - 21p_3^3p_4 - 28p_2p_3p_4^2 + 14p_1p_4^3 + 7p_3^2p_4^3\right.\\
&\qquad \left.-14p_2p_4^4 + 7p_3p_4^5 - p_4^7\right)/3\\
\hat{P}_{12}(p) &= 16p_2^2 + 36p_1p_3 - 6p_3^3 + 36p_1p_4^2 - 18p_3^2p_4^2 - 32p_2p_4^3 + 18p_3p_4^4 - 2p_4^6\\
\hat{P}_{13}(p) &= 4\left(20p_2p_3 + 30p_1p_4 - 15p_3^2p_4 - 20p_2p_4^2 + 10p_3p_4^3 - p_4^5\right)/3\\
\hat{P}_{22}(p) &= 3\left(20p_2p_3 + 30p_1p_4 - 15p_3^2p_4 - 20p_2p_4^2 + 10p_3p_4^3 - p_4^5\right)/2\\
\hat{P}_{23}(p) &= 24p_1\\
\hat{P}_{33}(p) &= 16p_2
\end{aligned} \tag{74}$$

and after the following MIBT:

$$\begin{aligned}
p'_1 &= 110\,592p_1 - 55\,296p_3^2 - 138\,240p_2p_4 + 98\,496p_3p_4^2 - 15\,066p_4^4\\
p'_2 &= 2304p_2 - 2592p_3p_4 + 612p_4^3\\
p'_3 &= 48p_3 - 21p_4^2
\end{aligned} \tag{75}$$

one obtains, for $p'_4 = 1$, the matrix R of class E3($s = 1$), reported in II:

$$\begin{aligned}
R'_{11}(\tilde{p}') &= 2p'_1(p'_2 - 54) + 15{p'_2}^2 + 216p'_2p'_3 + 324(4{p'_3}^2 + 18p'_3 + 81)\\
R'_{12}(\tilde{p}') &= 6p'_1p'_3 - {p'_2}^2 + 18p'_2(p'_3 + 12) + 1620p'_3\\
R'_{13}(\tilde{p}') &= 6p'_1 - p'_2(p'_3 - 27) + 54p'_3\\
R'_{22}(\tilde{p}') &= 4\left[3p'_1 - p'_2(p'_3 + 9) + 27({p'_3}^2 - 2p'_3 + 27)\right]\\
R'_{23}(\tilde{p}') &= p'_1 - 3p'_2 - 6{p'_3}^2 + 108p'_3\\
R'_{33}(\tilde{p}') &= p'_2 - 12p'_3 + 81\,.
\end{aligned} \tag{76}$$

3.11. Type D_4

The group acts on $x = (x_1, x_2, x_3, x_4)$ by permutations and by changes of an even number of signs of the coordinates. A MIB can be chosen as follows:

$$p_1(x) = \sum_1^4{}_i x_i^6 \qquad p_2(x) = \sum_1^4{}_i x_i^4 \qquad p_3(x) = \prod_{i=1}^4 x_i \qquad p_4(x) = \sum_1^4{}_i x_i^2\,. \tag{77}$$

The essential elements of the associated $\hat{P}$-matrix turn out to be the following:

$$\begin{aligned}
\hat{P}_{11}(p) &= 6(5p_1p_2 - 30p_3^2p_4 + 5p_1p_4^2 - 5p_2p_4^3 + p_4^5)\\
\hat{P}_{12}(p) &= 4(3p_2^2 - 24p_3^2 + 8p_1p_4 - 6p_2p_4^2 + p_4^4)\\
\hat{P}_{13}(p) &= 6p_2p_3\\
\hat{P}_{22}(p) &= 16p_1\\
\hat{P}_{23}(p) &= 4p_3p_4\\
\hat{P}_{33}(p) &= \left(2p_1 - 3p_2p_4 + p_4^3\right)/6
\end{aligned} \tag{78}$$

and, after the following MIBT:

$$p'_1 = 12\left(12p_1 - 15p_2p_4 + 4p_4^3\right) \qquad p'_2 = 48\sqrt{3}p_3 \qquad p'_3 = 6\left(-2p_2 + p_4^2\right) \tag{79}$$

one obtains, for $p'_4 = 1$, the matrix R of class E2($s = 1$), reported in II:

$$\begin{array}{ll} R'_{11}(\tilde{p}') = -4p'_1 + 5{p'_2}^2 + 5{p'_3}^2 + 12 & R'_{12}(\tilde{p}') = 2p'_2(p'_3 + 3) \\ R'_{13}(\tilde{p}') = {p'_2}^2 - p'_3(p'_3 - 6) & R'_{22}(\tilde{p}') = p'_1 + 3p'_3 + 6 \\ R'_{23}(\tilde{p}') = 3p'_2 & R'_{33}(\tilde{p}') = p'_1 - 3p'_3 + 6\,. \end{array} \tag{80}$$

3.12. Type F_4

The group is the group generated by all the reflections in $\mathbb{R}^4$ which leave invariant the hyperplanes $x_2 - x_3 = 0$, $x_3 - x_4 = 0$, $x_4 = 0$ and $x_1 - x_2 - x_3 - x_4 = 0$.

Let us define, for $r = 2, 6, 8, 12$:

$$\begin{aligned} S_k(x) &= \sum_1^k {}_i x_i^k \\ I_r(x) &= (8 - 2^{r-1})S_r + \sum_1^{r/2-1} {}_j \binom{r}{2j} S_{2j} S_{r-2j} \\ &= \sum_{1\leqslant i<j\leqslant 4} [(x_j + x_i)^r + (x_i - x_j)^r]\,. \end{aligned} \tag{81}$$

Then, according to Metha, a MIB for the group can be defined to be the following:

$$p_1(x) = I_{12}(x) \qquad p_2(x) = I_8(x) \qquad p_3(x) = I_6(x) \qquad p_4(x) = I_2(x)/6 \tag{82}$$

or, explicitly,

$$\begin{aligned} p_1(x) &= 924(x_1^6 + x_2^6 + x_3^6 + x_4^6)^2 + 990(x_1^4 + x_2^4 + x_3^4 + x_4^4)(x_1^8 + x_2^8 + x_3^8 + x_4^8) + 132(x_1^2 \\ &\quad + x_2^2 + x_3^2 + x_4^2)(x_1^{10} + x_2^{10} + x_3^{10} + x_4^{10}) - 2040(x_1^{12} + x_2^{12} + x_3^{12} + x_4^{12}) \\ p_2(x) &= 70(x_1^4 + x_2^4 + x_3^4 + x_4^4)^2 + 56(x_1^2 + x_2^2 + x_3^2 + x_4^2)(x_1^6 + x_2^6 + x_3^6 + x_4^6) - 120(x_1^8 \\ &\quad + x_2^8 + x_3^8 + x_4^8) \\ p_3(x) &= 30(x_1^2 + x_2^2 + x_3^2 + x_4^2)(x_1^4 + x_2^4 + x_3^4 + x_4^4) - 24(x_1^6 + x_2^6 + x_3^6 + x_4^6) \\ p_4(x) &= x_1^2 + x_2^2 + x_3^2 + x_4^2\,. \end{aligned} \tag{83}$$

The essential elements of the associated $\hat{P}(p)$ matrix turn out to be the following:

$$\begin{aligned} \hat{P}_{11}(p) &= \big(18\,711 p_2^2 p_3 + 1\,015\,740 p_1 p_2 p_4 - 10\,178\,010 p_2 p_3^2 p_4 - 625\,680 p_1 p_3 p_4^2 \\ &\quad + 12\,496 p_3^3 p_4^2 - 1\,675\,080 p_2^2 p_4^3 - 5\,264\,820 p_2 p_3 p_4^4 + 24\,793\,560 p_1 p_4^5 \\ &\quad + 14\,410\,440 p_3^2 p_4^5 - 254\,481\,480 p_2 p_4^7 + 470\,719\,260 p_3 p_4^8 - 1\,709\,728\,560 \\ &\quad p_4^{11}\big)/810 \\ \hat{P}_{12}(p) &= 4\big(11\,970 p_1 p_3 - 610 p_3^3 + 49\,977 p_2^2 p_4 - 175\,059 p_2 p_3 p_4^2 + 428\,220 p_1 p_4^3 \\ &\quad + 110\,052 p_3^2 p_4^3 - 4\,455\,270 p_2 p_4^5 + 9\,531\,630 p_3 p_4^6 - 32\,435\,640 p_4^9\big)/405 \\ \hat{P}_{13}(p) &= 4\big(243 p_2^2 + 2259 p_2 p_3 p_4 + 15\,480 p_1 p_4^2 - 5572 p_3^2 p_4^2 - 129\,240 p_2 p_4^4 \\ &\quad + 278\,250 p_3 p_4^5 - 847\,260 p_4^8\big)/45 \\ \hat{P}_{22}(p) &= 16\big(21 p_2 p_3 + 84 p_1 p_4 - 28 p_3^2 p_4 - 840 p_2 p_4^3 + 1890 p_3 p_4^4 - 6120 p_4^7\big)/3 \\ \hat{P}_{23}(p) &= 32\big(18 p_1 + 7 p_3^2 - 63 p_2 p_4^2 + 273 p_3 p_4^3 - 1134 p_4^6\big)/9 \\ \hat{P}_{33}(p) &= 72\big(-12 + p_2 p_4 + 4 p_3 p_4^2\big) \end{aligned} \tag{84}$$

and, after the following MIBT:

$$
\begin{aligned}
p'_1 &= 96\sqrt{6}\left(288p_1 - 77p_3^2 - 3762p_2p_4^2 + 8832p_3p_4^3 - 29\,511p_4^6\right)/5 \\
p'_2 &= 108\left(16p_2 - 56p_3p_4 + 255p_4^4\right)/5 \\
p'_3 &= 6\sqrt{6}\left(2p_3 - 15p_4^3\right)
\end{aligned}
\tag{85}
$$

one obtains, for $p'_4 = 1$, the matrix R of class E4 ($s = 1$), reported in II:

$$
\begin{aligned}
R'_{11}(\tilde{p}') &= -6\big[12p'_1p'_3 - 21{p'_2}^2 - p'_2(11{p'_3}^2 - 864) - 36(17{p'_3}^2 + 972)\big] \\
R'_{12}(\tilde{p}') &= -6\big[12p'_1 - p'_3(21p'_2 + {p'_3}^2 + 756)\big] \\
R'_{13}(\tilde{p}') &= {p'_2}^2 + 180p'_2 + 60{p'_3}^2 \\
R'_{22}(\tilde{p}') &= 6(9p'_2 + 7{p'_3}^2 + 972) \\
R'_{23}(\tilde{p}') &= p'_1 + 180p'_3 \\
R'_{33}(\tilde{p}') &= 5p'_2 + 324\,.
\end{aligned}
\tag{86}
$$

3.13. Type H_4

The group is defined as the group generated by all the reflections in $\mathbb{R}^4$ which leave invariant the hyperplanes $x_3 = 0$, $x_4 = 0$, $\tau^{-1}x_2 - \tau x_3 - x_4 = 0$ and $\tau^{-1}x_1 - \tau x_2 - x_4 = 0$, where τ is defined in (63).

For j, k, l, m in the set $\{1, 2, 3, 4\}$, let us define the following symbols:

$$
\eta_{jk} = \begin{cases} -1 & \text{for} \quad j = k \\ 1 & \text{otherwise} \end{cases}
\tag{87}
$$

and the following expressions:

$$
\xi(m, j, k, l; x) = \tau x_j\eta_{mj} + \tau^{-1}x_k\eta_{mk} + x_l\eta_{ml}\,;
\tag{88}
$$

$$
\chi(j, k, l, n; x) = \xi(0, j, k, l; x)^{2n} + \xi(j, j, k, l; x)^{2n} + \xi(k, j, k, l; x)^{2n} + \xi(l, j, k, l; x)^{2n}
\tag{89}
$$

$$
\psi(j, n; x) = \left(\sum_1^4{}_k\,\eta_{jk}x_k\right)^{2n}.
\tag{90}
$$

$$
\begin{aligned}
I_n(x) = {}& \sum_1^4{}_k(2x_k)^{2n} + \sum_0^4{}_k\psi(k; x) + \chi(1, 2, 3, n; x) + \chi(1, 3, 4, n; x) \\
& + \chi(1, 4, 2, n; x) + \chi(2, 4, 3, n; x)\,.
\end{aligned}
\tag{91}
$$

Then, according to Metha, a MIB for H_4 can be chosen in the following way:

$$
p_1(x) = I_{30}(x) \qquad p_2(x) = I_{20}(x) \qquad p_3(x) = I_{12}(x) \qquad p_4(x) = \sum_1^4{}_i\,x_i^2\,.
\tag{92}
$$

The essential elements of the associated $\hat{P}$-matrix turn out to be the following:

$$\begin{aligned}
\hat{P}_{11}(p) = {} & 53\,911 p_2 p_3^3 p_4/7616 + 7\,051\,785 p_1 p_3^2 p_4^2/56 + 4\,821\,334\,245 p_2^2 p_3 p_4^3/25\,432 \\
& + 2\,186\,873\,325 p_1 p_2 p_4^4/34 - 645\,826\,368\,707 p_3^4 p_4^5/150\,528 \\
& - 116\,309\,076\,672\,555 p_2 p_3^2 p_4^7/23\,936 - 211\,651\,127\,025 p_1 p_3 p_4^8/2 \\
& - 21\,238\,646\,708\,813\,625 p_2^2 p_4^9/18\,496 - 283\,066\,493\,617\,380\,915 p_3^3 p_4^{11}/9856 \\
& - 2\,811\,241\,304\,150\,172\,075 p_2 p_3 p_4^{13}/544 + 2\,218\,140\,033\,302\,250 p_1 p_4^{14} \\
& + 7\,676\,790\,020\,731\,375\,739\,325 p_3^2 p_4^{17}/224 \\
& - 15\,228\,773\,425\,368\,084\,479\,625 p_2 p_4^{19}/136 \\
& + 253\,639\,342\,346\,876\,415\,408\,375 p_3 p_4^{23}/8 \\
& - 8\,927\,280\,781\,972\,196\,041\,680\,013\,125 p_4^{29}/4 \\
\hat{P}_{12}(p) = {} & 26\,741 p_3^4/61\,740 + 2\,357\,459 p_2 p_3^2 p_4^2/56 + 1\,473\,900 p_1 p_3 p_4^3 + 482\,714\,505 p_2^2 p_4^4/22 \\
& - 1\,869\,793\,842\,241 p_3^3 p_4^6/7056 - 7\,474\,081\,897\,815 p_2 p_3 p_4^8/44 \\
& + 327\,790\,212\,400 p_1 p_4^9 + 66\,300\,758\,108\,151\,125 p_3^2 p_4^{12}/308 \\
& - 34\,964\,650\,402\,339\,275 p_2 p_4^{14} + 128\,303\,960\,304\,363\,056\,775 p_3 p_4^{18} \\
& - 993\,168\,612\,785\,995\,074\,523\,500 p_4^{24} \\
\hat{P}_{13}(p) = {} & 429\,975 p_2^2/3179 + 4\,236\,791 p_3^3 p_4^2/168 + 2\,490\,103\,980 p_2 p_3 p_4^4/187 \\
& + 92\,563\,800 p_1 p_4^5 - 7\,157\,961\,621\,135 p_3^2 p_4^8/88 - 330\,008\,206\,170\,825 p_2 p_4^{10}/34 \\
& + 36\,082\,213\,228\,297\,575 p_3 p_4^{14} - 271\,058\,613\,666\,147\,798\,750 p_4^{20} \\
\hat{P}_{22}(p) = {} & 2\,657\,644 p_3^3 p_4/138\,915 + 24\,894\,256 p_2 p_3 p_4^3/21 + 5\,074\,562\,560 p_1 p_4^4/819 \\
& - 1\,343\,036\,354\,024 p_3^2 p_4^7/441 - 644\,361\,278\,880 p_2 p_4^9 \\
& + 49\,357\,102\,179\,756\,800 p_3 p_4^{13}/21 - 4\,855\,838\,749\,013\,355\,171\,200 p_4^{19}/273 \\
\hat{P}_{23}(p) = {} & 10\,880 p_1/13 + 1\,322\,362 p_3^2 p_4^3/21 - 80\,135\,160 p_2 p_4^5 + 296\,137\,692\,080 p_3 p_4^9 \\
& - 29\,473\,265\,236\,173\,600 p_4^{15}/13 \\
\hat{P}_{33}(p) = {} & 5040 p_4 (7 p_2 - 18\,224 p_3 p_4^4 + 167\,747\,160 p_4^{10})/17
\end{aligned} \tag{93}$$

and, after the following MIBT:

$$\begin{aligned}
p_1' &= 98\,415\,000 \big(576 p_1/1001 - 108\,555 p_3^2 p_4^3/539 - 11\,535\,372 p_2 p_4^5/187 \\
&\qquad + 17\,469\,633\,928 p_3 p_4^9/77 - 1\,724\,135\,397\,013\,808 p_4^{15}/1001\big) \\
p_2' &= 2\,187\,000 \big(-6 p_2/187 + 1307 p_3 p_4^4/11 - 908\,706 p_4^{10}\big) \\
p_3' &= 1620 \big(-p_3/7 + 1130 p_4^6\big)
\end{aligned} \tag{94}$$

one obtains, for $p_4' = 1$, the matrix R of class E5 ($s = 1$) reported in II†:

$$\begin{aligned}
\hat{R}_{11}'(p') = {} & -36 p_2^2(-25\,380 + 19 p_3) + 90 p_1(-1\,166\,400 + 12 p_2 + 1\,080 p_3 + p_3^2) \\
& - p_2(-75\,582\,720\,000 - 342\,921\,600 p_3 - 6\,480 p_3^2 + 29 p_3^3) \\
& + 45(918\,330\,048\,000\,000 + 906\,992\,640\,000 p_3 + 1\,102\,248\,000 p_3^2 \\
& - 339\,120 p_3^3 + 209 p_3^4)
\end{aligned}$$

† In II, the sign of the monomial $p_1 p_3$ in the expression of R_{11}' is wrong and should be changed.

$$
\begin{aligned}
\hat{R}'_{12}(p') &= -486p_2^2 + 360p_1(540 + p_3) - 9p_2(-34\,992\,000 - 3\,240p_3 + 19p_3^2) \\
&\quad - p_3(-89\,754\,480\,000 + 28\,431\,000p_3 - 45\,360p_3^2 + p_3^3) \\
\hat{R}'_{13}(p') &= 2\,160p_1 + p_2^2 - 1\,980p_2(-1080 + p_3) - 55(-4860 + p_3)p_3^2 \\
\hat{R}'_{22}(p') &= 212\,576\,400\,000 + 540p_1 - 45\,927\,000p_3 + 218\,700p_3^2 - 19p_3^3 \\
&\quad - 324p_2(2025 + p_3) \\
\hat{R}'_{23}(p') &= p_1 - 810p_2 - 495(-2700 + p_3)p_3 \\
\hat{R}'_{33}(p') &= 11p_2 - 6\,750(-1296 + p_3)\,.
\end{aligned}
\tag{95}
$$

4. Reducible reflection groups with 2, 3 and 4 basic invariants

In this section we shall state the rules for building the $\hat{P}$-matrices of a reducible coregular linear group G, in a standard A-basis, starting from the $\hat{P}$-matrices associated to its irreducible components. This will allow us, in particular, to derive the explicit form of the $\hat{P}$-matrices of all the reducible reflection groups whose orbit spaces have dimensions $\leqslant 4$ and state which of the allowable $\hat{P}$-matrices determined in I and II are related to these groups.

Let $G^{(1)}$ and $G^{(2)}$ be irreducible CLGs, acting, respectively, in $\mathbb{R}^{n_1}$ and $\mathbb{R}^{n_2}$. Then, the set of matrices

$$
G = \{g^{(1)} \oplus g^{(2)}\}_{\substack{g^{(\alpha)} \in G^{(\alpha)} \\ \alpha = 1,2}} \tag{96}
$$

forms a coregular linear group, acting on the vectors $x = x^{(1)} \oplus x^{(2)},\ x \in \mathbb{R}^{n_1+n_2} = \mathbb{R}^{n_1} \oplus \mathbb{R}^{n_2}$. If the groups $G^{(\alpha)},\ \alpha = 1, 2$ are generated by reflections, G is a reflection group isomorphic to $G_1 \otimes G_2$.

Let us denote by $p_i^{(\alpha)}(x^{(\alpha)}),\ i = 1, \ldots, q_\alpha,\ x^{(\alpha)} \in \mathbb{R}^{n_\alpha}$ the elements of a standard MIB relative to $G^{(\alpha)},\ \alpha = 1, 2$ and by $\{d_i^{(\alpha)}\},\ \hat{P}^{(\alpha)}(p^{(\alpha)})$ the associated set of degrees and $\hat{P}$-matrix. We shall assume $d_1^{(1)} \geqslant d_1^{(2)}$.

A set of basic polynomial invariants of G is yielded by

$$
p^{(+)}(x) = \{p^{(1)}(x^{(1)}), p^{(2)}(x^{(2)})\} \tag{97}
$$

and the associated $\hat{P}$-matrix has the following form:

$$
\hat{P}^{(+)}(p^{(+)}) = \hat{P}^{(1)}(p^{(1)}) \oplus \hat{P}^{(2)}(p^{(2)})\,. \tag{98}
$$

If $\{p^{(\alpha)}\}$ is a standard A-basis relative to $G^{(\alpha)}$, $A^{(\alpha)}(p^{(\alpha)})$ is the complete active factor of $\det \hat{P}^{(\alpha)}(p^{(\alpha)})$ and $w^{(\alpha)}$ is its weight, then

$$
A^{(+)}(p^{(+)}) = A^{(1)}(p^{(1)})A^{(2)}(p^{(2)}) \tag{99}
$$

is the complete active factor of $\det \hat{P}^{(+)}$; it satisfies the following relations:

$$
\sum_{1}^{q_1+q_2}{}_b\, \hat{P}_{ab}^{(+)}(p^{(+)})\partial_b A^{(+)}(p^{(+)}) = \lambda_a^{(+)} A^{(+)}(p^{(+)}) \qquad a = 1, \ldots, q_1 + q_2 \tag{100}
$$

where

$$
\lambda^{(+)} = \lambda^{(1)} \oplus \lambda^{(2)} = (0, \ldots, 0, 2w^{(1)}, 0, \ldots, 0, 2w^{(2)})\,. \tag{101}
$$

Therefore, a standard A-basis $\{p\}$ of G can be obtained from $\{p^{(+)}\}$ by means of a basis transformation $p = f(p^{(+)})$, with $f(p^{(+)})$ defined, for instance, by the following relations:

$$\begin{aligned} p_k &= p^{(+)}_{i(k)} \qquad k = 1, \ldots, q_1 + q_2 - 2 \\ p_{q_1+q_2-1} &= b_{q_1+q_2-1}\big(w^{(2)} p^{(1)}_{q_1} - w^{(1)} p^{(2)}_{q_2}\big) \\ p_{q_1+q_2} &= p^{(1)}_{q_1} + p^{(2)}_{q_2} \end{aligned} \tag{102}$$

in (102), the set $\{i(1), \ldots, i(q_1+q_2-2)\}$ is a permutation of the indices $\{1, \ldots, q_1+q_2-2\}$, such that the degrees of the invariants p_k are non increasing functions of k. The parameters b_k are arbitrary and will be chosen so that the $\hat{P}$-matrices can be easily compared with the results reported in I and II.

The $\hat{P}$-matrix associated to the MIB $\{p\}$ is determined by the following relation (see equation (15)):

$$\hat{P}(p) = J(p^{(+)})\, \hat{P}^{(+)}(p^{(+)})\, J^T(p^{(+)})\Big|_{p^{(+)}=f^{-1}(p)} \tag{103}$$

where $J(p^{(+)})$ denotes the Jacobian matrix

$$J_{ab}(p^{(+)}) = \frac{\partial f_a(p^{(+)})}{\partial p^{(+)}_b} \qquad a, b = 1, \ldots, q_1 + q_2\,. \tag{104}$$

In the aim of determining the $\hat{P}$-matrices of all the reducible reflection groups whose orbit spaces have dimensions 3 and 4, let us now specialize the construction we have described to the cases $q_1 = 2,\ q_2 = 1, 2$ and to each of the different cases one can get starting from $q_1 = 3,\ q_2 = 1$. We shall denote by w the weight of the complete active factor $A(p)$ of $\det \hat{P}(p)$:

$$w = w^{(+)} = w^{(1)} + w^{(2)}\,. \tag{105}$$

Below, for each of the different reducible groups that can be obtained in this way, we shall list the values of the degrees, the explicit form of the matrix $R^{(+)}$, the MIBT leading to a standard A-basis and the transformed form of the matrix $R(p)$, evaluated at $p_q = 1$, to be compared with the results of I and II.

4.1. Case $q_1 = 2,\ q_2 = 1$

$$\begin{aligned} &d_1 = d^{(1)}_1 = m + 1 \qquad d_3 = d^{(2)}_1 = 2 \\ &d_2 = d^{(1)}_2 = 2 \qquad\quad\;\; w = 2d^{(1)}_1 + 2 = 2m + 4 \end{aligned} \qquad m \in \mathbb{N}_* \tag{106}$$

$$\begin{aligned} &R^{(+)}_{11}(p^{(+)}) = p^{(1)m}_2 \qquad R^{(+)}_{a3}(p^{(+)}) = 0 \qquad a = 1, 2 \\ &R^{(+)}_{12}(p^{(+)}) = p^{(1)}_1 \qquad R^{(+)}_{33}(p^{(+)}) = p^{(2)}_1 \\ &R^{(+)}_{22}(p^{(+)}) = p^{(1)}_2 \qquad R^{(+)}_{44}(p^{(+)}) = p^{(2)}_2 \end{aligned} \tag{107}$$

$$p_1 = (2+m)^{m/2} p^{(1)}_1 \qquad p_2 = -p^{(1)}_2 + (m+1) p^{(2)}_1 \qquad p_3 = p^{(1)}_2 + p^{(2)}_1 \tag{108}$$

$$\begin{aligned} &R_{11}(p) = \big[(1+m)p_3 - p_2\big]^m \qquad R_{22}(p) = (1+m)p_3 + m p_2 \\ &R_{12}(p) = -p_1 \qquad\qquad\qquad\quad\;\; R_{a3}(p) = p_a \qquad a = 1, 2, 3 \end{aligned} \tag{109}$$

which, for $p_3 = 1$, is the class II R-matrix reported in II.

4.2. Case $q_1 = 2,\ q_2 = 2$

$$\begin{array}{ll} d_1 = d_1^{(1)} = j_1 + 1 & d_3 = d_2^{(1)} = 2 \\ d_2 = d_1^{(2)} = j_2 + 1 & d_4 = d_2^{(2)} = 2 \end{array} \qquad j_1, j_2 \in \mathbb{N}_* \tag{110}$$

$$w = w^{(1)} + w^{(2)} = 2(j_1 + j_2 + 2) \tag{111}$$

$$\begin{array}{lll} R_{11}^{(+)}(p^{(+)}) = p_2^{(1)\,j_1} & R_{22}^{(+)}(p^{(+)}) = p_2^{(1)} & R_{34}^{(+)}(p^{(+)}) = p_1^{(2)} \\ R_{12}^{(+)}(p^{(+)}) = p_1^{(1)} & R_{33}^{(+)}(p^{(+)}) = p_2^{(2)\,j_2} & R_{44}^{(+)}(p^{(+)}) = p_2^{(2)} \\ R_{ab}^{(+)}(p^{(+)}) = 0 & a = 1, 2 \qquad b = 3, 4 & \end{array} \tag{112}$$

$$\begin{array}{ll} p_1 = (j_1 + j_2 + 2)^{j_1/2} p_1^{(1)} & p_3 = (j_2 + 1) p_2 - (j_1 + 1) p_4 \\ p_2 = (j_1 + j_2 + 2)^{j_1/2} p_1^{(2)} & p_4 = p_2^{(1)} + p_2^{(2)} \end{array} \tag{113}$$

$$\begin{array}{ll} R_{11}(p) = (j_1 + j_2 + 2)[-p_3 + (j_1 + 1) p_4]^{j_1} & R_{12}(p) = 0 \\ R_{22}(p) = (j_1 + j_2 + 2)[p_3 + (j_2 + 1) p_4]^{j_2} & R_{13}(p) = -(j_2 + 1) p_1 \\ R_{33}(p) = (j_1 + 1)(j_2 + 1) + (j_1 - j_2) p_3 & R_{23}(p) = (j_1 + 1) p_2 \end{array} \tag{114}$$

which, for $p_3 = 1$, is the class A8(j_1, j_2) R-matrix reported in II. For $j_i = 1$ the group $G^{(i)} \simeq Z_2 \otimes Z_2$ is reducible.

4.3. Cases $q_1 = 3,\ q_2 = 1$

$$\begin{array}{ll} d_1 = d_1^{(1)} & d_3 = d_3^{(1)} \\ d_2 = d_2^{(1)} & d_4 = d_1^{(2)} \end{array} \qquad w = w^{(1)} + 2 \tag{115}$$

$$\begin{array}{ll} R^{(+)}(p^{(+)})_{ab} = R_{ab}^{(1)}(p^{(1)}) & a, b = 1, 2, 3 \\ R^{(+)}(p^{(+)})_{a4} = 0 & a = 1, 2, 3 \\ R^{(+)}(p^{(+)})_{44} = R_{11}^{(2)}(p^{(2)}) = p_1^{(2)} & \end{array} \tag{116}$$

$$p_1 = b_1 p_1^{(1)} \qquad p_3 = b_3\big(p_3^{(1)} - w^{(1)} p_1^{(2)}/2\big) p_2 = b_2 p_2^{(1)} \qquad p_4 = p_3^{(1)} + p_1^{(2)}\,. \tag{117}$$

The matrix $R^{(1)}$ can be chosen from three different classes, denoted as III.1, III.2, III.3 in II and corresponding, respectively, to the groups of type A_3 (or D_3), B_3 and H_3.

Choosing as $G^{(1)}$ a type A_3 group one obtains:

$$\begin{array}{ll} d_1 = 4 & d_3 = d_4 = 2 \\ d_2 = 3 & w^{(1)} = 12 \end{array} \tag{118}$$

$$\begin{array}{ll} p_1 = 49 p_1^{(1)} & p_3 = p_3^{(1)} - 6 p_1^{(2)} \\ p_2 = -7^{3/2} p_2^{(1)} & p_4 = p_3^{(1)} + p_1^{(2)} \end{array} \tag{119}$$

$$\begin{array}{l} R_{11}(p) = 7\big[p_2^2 - p_1(p_3 + 6p_4) + 2(p_3 + 6p_4)^3\big] \\ R_{22}(p) = 7\big[p_1 + 2(p_3 + 6p_4)^2\big] \\ R_{12}(p) = 14 p_2 (p_3 + 6p_4) \\ R_{13}(p) = p_1 \qquad R_{23}(p) = p_2 \qquad R_{33}(p) = -5p_3 + 6p_4 \end{array} \tag{120}$$

which, for $p_4 = 1$, is the class B4$(s = 1)$ R-matrix reported in II.

Choosing as $G^{(1)}$ a type B_3 group one obtains:

$$\begin{aligned} &d_1 = 6 \qquad d_3 = d_4 = 2 \\ &d_2 = 4 \qquad w^{(1)} = 18 \end{aligned} \tag{121}$$

$$\begin{aligned} &p_1 = 10^3 p_1^{(1)} \qquad p_3 = p_3^{(1)} - 9p_1^{(2)} \\ &p_2 = -10^2 p_2^{(1)} \qquad p_4 = p_3^{(1)} + p_1^{(2)} \end{aligned} \tag{122}$$

$$\begin{aligned} &R_{11}(p) = 10\left\{p_1\left[p_2 - 4(p_3+9p_4)^2\right] + 8(p_3+9p_4)\left[p_2^2 + 2p_2(p_3+9p_4)^2 + 8(p_3+9p_4)^4\right]\right\} \\ &R_{12}(p) = 10\left\{2p_1(p_3+9p_4) - p_2\left[p_2 - 12(p_3+9p_4)^2\right]\right\} \\ &R_{22}(p) = 10\left\{p_1 - 4(p_3+9p_4)\left[p_2 - 4(p_3+9p_4)^2\right]\right\} \\ &R_{13}(p) = p_1 \qquad R_{23}(p) = p_2 \qquad R_{33}(p) = -8p_3 + 9p_4 \end{aligned} \tag{123}$$

which, for $p_4 = 1$, is the class C6(1) R-matrix reported in II.

Choosing as $G^{(1)}$ a type H_3 group one obtains:

$$\begin{aligned} &d_1 = 10 \qquad d_3 = d_4 = 2 \\ &d_2 = 6 \qquad w^{(1)} = 30 \end{aligned} \tag{124}$$

$$\begin{aligned} &p_1 = 16^5 p_1^{(1)} \qquad p_3 = p_3^{(1)} - 15p_1^{(2)} \\ &p_2 = -16^3 p_2^{(1)} \qquad p_4 = p_3^{(1)} + p_1^{(2)} \end{aligned} \tag{125}$$

$$\begin{aligned} R_{11}(p) = 16\Big\{&4p_1(p_3+15p_4)\left[p_2 - 3(p_3+15p_4)^3\right] - \left[p_2 - 48(p_3+15p_4)^3\right] \\ &\times\left[p_2^2 + 4p_2(p_3+15p_4)^3 + +24(p_3+15p_4)^6\right]\Big\} \end{aligned} \tag{126}$$

$$\begin{aligned} &R_{12}(p) = 16(p_3+15j_1p_4)\left[-5p_2^2 + 6p_1(p_3+15p_4) + 60p_2(p_3+15p_4)^3\right] \\ &R_{22}(p) = 16\left[p_1 - 14p_2(p_3+15p_4)^2 + 96(p_3+15p_4)^5\right] \\ &R_{13}(p) = p_1 \qquad R_{23}(p) = p_2 \qquad R_{33}(p) = -14p_3 + 15p_4 \end{aligned} \tag{127}$$

which, for $p_4 = 1$, is the class D4(j_1) R-matrix reported in II.

5. Concluding remarks on the mathematical results

Starting from explicit forms for the basic polynomial invariants of the finite coregular groups, that can be found in the mathematical literature, we have computed the associated $\hat{P}(p)$ matrices. The equalities and inequalities, defining the orbit spaces of the groups as semi-algebraic sub-varieties of $\mathbb{R}^q$, can be easily obtained as semi-positivity conditions on these matrices.

The computation has been limited to the coregular groups with less than five basic polynomial invariants, since the main aim of our work was to test the completeness of the allowable solutions of the canonical equation listed in I and II and to find the corresponding generating groups. The test has been positive: all the $\hat{P}$-matrices generated by finite coregular groups appear in the lists of allowable $\hat{P}$-matrices reported in I and II. In particular,

(i) For $q = 2$ all the allowable $\hat{P}$-matrices are generated by coregular *finite* groups; the case $q = 2$ is exceptional, since the canonical equation puts no restrictions on the allowable $\hat{P}$-matrices. On the contrary, for $q = 3, 4$, only the fundamental elements (scale parameter $s = 1$) of some towers of allowable $\hat{P}$-matrices are generated by coregular *finite* groups; in this case, the existence of towers of solutions of the canonical equation probably has no group-theoretical meaning, but is only an artefact related to an invariance of the canonical equation under scaling of the degrees of the basic polynomial invariants. By now, however, we cannot exclude that the higher elements in the towers are generated by non-finite groups.

(ii) For $q = 2, 3, 4$ all the *fully active* allowable solutions of the canonical equation are generated by *finite* coregular linear groups; the *irreducible* ones are associated to *irreducible* linear groups.

As for the fundamental allowable $\hat{P}$-matrices for which we have not found a finite coregular generating group, various, more or less obvious, interpretations are possible; they might be generated by

(i) non-finite compact coregular groups,
(ii) non-coregular groups,
(iii) non-minimal integrity bases of finite or non-finite compact coregular groups,
(iv) direct sums of non-fundamental allowable $\hat{P}$-matrices.

This is probably an incomplete list.

We shall try to clarify this point in two forthcoming papers. The correspondence between the classification of the allowable $\hat{P}$-matrices determined in I and II and the generating finite reflection groups with less than five basic polynomial invariants is summarized in tables 1–4, where by a group of type $I_2(1)$ we mean the group $Z_2 \otimes Z_2$, ($Z_2 = \{\pm 1\}$). The case $q = 1$ is trivial, as there is only one allowable $\hat{P}$-matrix generated by the group Z_2. For $q = 2$, for each choice of the degree d_1 there is only one equivalence class of allowable $\hat{P}$-matrices, which are generated by at least one finite coregular linear group. For $q = 3$, all the fundamental elements in each tower of (classes of) allowable solutions are generated by at least one finite coregular group, but for the $\hat{P}$-matrices of class I. For $q = 4$, the number of (classes of) reducible allowable solutions which are not generated by at least one finite coregular group is much higher.

Table 1. Correspondence between classes of allowable solutions of the canonical equation (labelled by the degree d_1) and finite coregular generating groups, for $q = 2$.

Group	$Z_2 \otimes Z_2$	$A_2,\ I_2(3)$	$B_2,\ I_2(4)$	$I_2(5)$	$G_2,\ I_2(6)$	$I_2(m)$
d_1	2	3	4	5	6	$m > 6$

Table 2. Correspondence between classes of fundamental allowable solutions of the canonical equation, degrees of the basic invariants and finite coregular generating groups, for $q = 3$.

Group	$I_2(m+1) \otimes Z_2$	$A_3,\ D_3$	B_3	H_3
(d_1, d_2)	$(m+1, 2)$	$(4, 3)$	$(6, 4)$	$(10, 6)$
Class	II(m), $m \in \mathbb{N}_*$	III.1	III.2	III.3

Table 3. Correspondence between classes of irreducible fundamental allowable solutions of the canonical equation, degrees of the basic invariants and finite coregular irreducible generating groups, for $q = 4$.

Group	A_4	D_4	B_4	F_4	H_4
(d_1, d_2, d_3)	$(5, 4, 3)$	$(6, 4, 4)$	$(8, 6, 4)$	$(12, 8, 6)$	$(30, 20, 12)$
Class	E1	E2	E3	E4	E5

Table 4. Correspondence between classes of reducible fundamental allowable solutions of the canonical equation, degrees of the basic invariants and finite coregular reducible generating groups, for $q = 4$.

Group	$I_2(j_1+1)\otimes I_2(j_2+1)$	$A_3\otimes Z_2$, $D_3\otimes Z_2$	$B_3\otimes Z_2$	$H_3\otimes Z_2$
(d_1, d_2, d_3)	$((j_1+1), (j_2+1), 2)$	(4, 3, 2)	(6, 4, 2)	(10, 6, 2)
Class	$\mathrm{A8}(j_1, j_2)$, $j_1 \geqslant j_2 \in \mathbb{N}_*$	B4(1)	C6(1)	D4(1)

6. Physical applications. An example

The $\hat{P}$ matrix approach to the study of orbit spaces has been, or can be used, in various physical contexts, where the study of covariant functions is important, as already stressed in the introduction. Typical examples are the determination of patterns of spontaneous symmetry and/or supersymmetry breaking [20, 7] in gauge-field theories of elementary particles, the analysis of phase spaces and structural phase transitions in the framework of Landau's theory [49, 50] and in cosmology (phase transitions in the hot Universe [51]). Applications can be found in covariant bifurcation theory [52] or in crystal field theory and in most areas of solid state theory where use is made of symmetry adapted functions.

Most of the groups dealt with in the preceding sections are crystallographic groups, they are therefore symmetry groups of regular polyhedra in two, three or four dimensions and of root diagrams of simple Lie algebras. In particular, $I_2(m)$ denotes, in Coxeter's notation, the dihedral group denoted by C_{nv} in the standard physical notation [49], $I_2(m)\otimes\mathbb{Z}_2$ denotes D_{nh}, while D_3, B_3 and H_3 correspond, respectively, to the groups T_d, O_h and Y_h; F_4 is the symmetry group of a regular solid in $\mathbb{R}^4$ with 24 three-dimensional octahedral faces; H_4 is the symmetry group of a regular solid in $\mathbb{R}^4$ with 120 three-dimensional dodecahedral faces or, dually, of a regular 600-sided solid with tetrahedral faces; the groups A_3, A_4, B_4 and D_4 are strictly related to permutation groups or semi-direct products of permutation groups and sign change groups, as explained in section 3.

Solid state physics is, therefore, a natural physical context where our results can be exploited. As an example of the use of the $\hat{P}$-matrix approach to the analysis of properties of an invariant function, and, in particular, of the determination of the location of its stationary points and of its absolute minimum, in this section we shall study a six-degree expansion of a Landau thermodynamic potential $G(x;\pi,T)$, which depends on the vector valued order parameter $x = (x_1, x_2, x_3)$, transforming according to the fundamental representation of the group O_h. At the end we shall restrict our results to $BaTiO_3$ and determine its phase space using an oversimplified expression for its free energy.

6.1. The orbit space of the group O_h and its stratification

In the Coxeter notations used in the preceding sections, the fundamental representation of the group O_h corresponds to the group B_3, for which an MIB is specified in (56) and the corresponding $\hat{P}$-matrix in (57) and (13), with $d_1 = 6$, $d_2 = 4$, $d_3 = 2$.

To describe the geometry of the image $\bar{\mathcal{S}}$ of the orbit space of O_h, let us define the following auxiliary polynomial functions of p:

$$
\begin{aligned}
&f_1(p) = -p_2 + p_3^2 \qquad f_2(p) = -p_1 + p_3^3 \\
&f_3(p) = 3p_2 - p_3^2 \qquad f_4(p) = 9p_1 - p_3^3 \qquad f_5(p) = 2p_2 - p_3^2
\end{aligned}
\tag{128}
$$

$$f_6(p) = 4p_1 - p_3^3 \qquad f_7(p) = p_3^3 - 3p_3p_2 + 2p_1$$
$$f_8(p) = -p_3^6 + 9p_2p_3^4 - 8p_1p_3^3 - 21p_2^2p_3^2 + 36p_1p_2p_3 + 3p_2^3 - 18p_1^2\,.$$

The shape and primary stratification of $\bar{\mathcal{S}}$ can be immediately deduced from an inspection of the condition

$$\det \hat{P}(p) = f_7(p)f_8(p) = 0 \tag{129}$$

the results obtained in this way are confirmed by a complete analysis of the positivity and rank conditions on the matrix $\hat{P}(p)$ defined in (57). The section Ξ of the orbit space with the plane p_3 =consantt is plotted in figure 1, where the axes are labelled by the adimensional variables

$$u = p_2/p_3^2 \qquad v = p_1/p_3^3\,. \tag{130}$$

The determination of the isotropy type stratification of $\bar{\mathcal{S}}$, that is the determination of the orbit types of the different primary strata, requires a sounder analysis: for a convenient choice of the point $\bar{p}$ in each stratum, one has first to find a solution $\bar{x} = (\bar{x}_1, \bar{x}_2, \bar{x}_3)$ of the following equations†:

$$x_1^6 + x_2^6 + x_3^6 = \bar{p}_1 x_1^4 + x_2^4 + x_3^4 = \bar{p}_2 x_1^2 + x_2^2 + x_3^2 = \bar{p}_3 \tag{131}$$

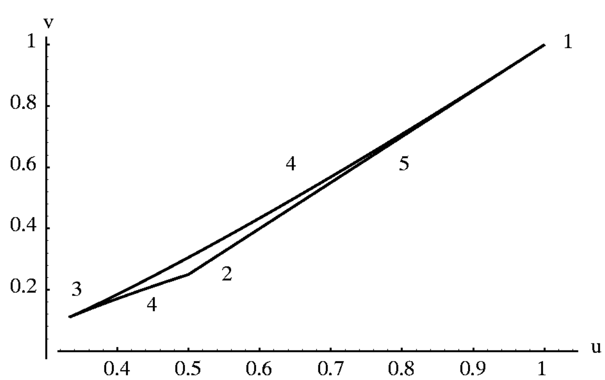

Figure 1. Stratification of the orbit space of the group O_h. The numbers j, $j = 1, \ldots 5$, label the singular isotropy type strata Σ_j defined in table 5.

and then, to determine the isotropy subgroup of O_h at $\bar{x}$, by selecting the transformations of O_h which leave $\bar{x}$ invariant.

A solution $\bar{x}$ of (131) for each stratum is easily found by noting that

$$\begin{aligned}\det \hat{P}(p(x)) &= f_7(p(x))f_8(p(x)) \\ &= 36x_1^2x_2^2x_3^2(x_1^2 - x_2^2)^2(x_2^2 - x_3^2)^2(x_3^2 - x_1^2)^2.\end{aligned} \tag{132}$$

The results one obtains are reported in table 5.

† The numbers $(\bar{x}_1, \bar{x}_2, \bar{x}_3)$ are the non-negative solutions of the real equation $\sum_{0_k}^3 a_k z^k = 0$, with $a_0 = (-\bar{p}_3^3 + 2\bar{p}_2\bar{p}_3 - 2\bar{p}_1)/6$ $(= -\bar{x}_1^2\bar{x}_2^2\bar{x}_3^2)$, $a_1 = (\bar{p}_3^2 - \bar{p}_2)/2$ $(= \bar{x}_1^2\bar{x}_2^2 + \bar{x}_2^2\bar{x}_3^2 + \bar{x}_3^2\bar{x}_1^2)$, $a_2 = \bar{p}_3$ $(= \bar{x}_1^2 + \bar{x}_2^2 + \bar{x}_3^2)$, $a_3 = 1$.

Table 5. Isotropy type strata of the orbit space of the 3-dimensional representation of the group O_h.

Strata	Defining relations in $\mathbb{R}^q$	Typical points in $\mathbb{R}^n$
$\Sigma_0 = \{O_h\}$	$p_1 = p_2 = p_3 = 0$	$\bar{x}_1 = \bar{x}_2 = \bar{x}_3 = 0$
$\Sigma_1 = \{C_{4v}\}$	$f_1 = f_2 = 0 < p_3$	$\bar{x}_1 = 1,\ \bar{x}_2 = \bar{x}_3 = 0$
$\Sigma_3 = \{C_{3v}\}$	$f_3 = f_4 = 0 < p_3$	$\bar{x}_1 = \bar{x}_2 = \bar{x}_3 = 1$
$\Sigma_2 = \{C_{2v}\}$	$f_5 = f_6 = 0 < p_3$	$\bar{x}_1 = 0,\ \bar{x}_2 = \bar{x}_3 = 1$
$\Sigma_4 = \{C_s'\}$	$f_8 = 0 < f_3, f_7, p_3$	$\bar{x}_1 = 1,\ \bar{x}_2 = \bar{x}_3 = 2$
$\Sigma_5 = \{C_s'\}$	$f_7 = 0 < f_1, f_5, p_3$	$\bar{x}_1 = 0,\ \bar{x}_2 = 1, \bar{x}_3 = 2$
$\Sigma_{\mathrm{p}} = \{C_1\}$	$0 < f_7, f_8, p_3$	$\bar{x}_1 = 1,\ \bar{x}_2 = 2,\ \bar{x}_3 = 3$

6.2. *The absolute minimum of the potential. Phase transitions*

Let us now build the potential

$$G(x; \pi, T) = \hat{G}(p(x); \pi, T) \tag{133}$$

as the most general sixth order O_h invariant polynomial function of the order parameters, the coefficients c, A_i and B_j being functions of the pressure π and the absolute temperature T:

$$\hat{G}(p; \pi, T) = \tfrac{1}{2}cp_3 + \tfrac{1}{4}(A_0 p_3^2 + A_1 p_2) + \tfrac{1}{6}(B_0 p_3^3 + B_1 p_3 p_2 + B_2 p_1)\,. \tag{134}$$

In order to assure stability of the system, we shall require that $G(x; \pi, T)$ is bounded below. This occurs if and only if the coefficient of p_3^3 in the asymptotic form of $\hat{G}$ for $p_3 \to \infty$:

$$C_{\mathrm{as}}(u, v) = \tfrac{1}{6}\,(B_0 + B_1 u + B_2 v) \tag{135}$$

is everywhere positive on Ξ, i.e. iff its minimum in Ξ is $>$ 0. Since the equation $C_{\mathrm{as}}(u, v) =$ constant defines straight lines in the plane (u, v) and $\bar{\mathcal{S}}$ is inscribed in a triangle with vertices at the points representing the strata $\{C_{iv}\}$, $i = 2, 3, 4$ (see figure 1), one easily realizes that $C_{\mathrm{as}}(u, v)$ is bound to take on its absolute minimum at at least one of the vertices. Therefore, $\hat{G}(p; \pi, T)$ is bounded below if and only if the following inequalities are satisfied:

$$\begin{aligned} C_{\mathrm{as}}(u, v)|_{\{C_{2v}\}} &= (4B_0 + 2B_1 + B_2)/4 > 0 \\ C_{\mathrm{as}}(u, v)|_{\{C_{3v}\}} &= (9B_0 + 3B_1 + B_2)/9 > 0 \\ C_{\mathrm{as}}(u, v)|_{\{C_{4v}\}} &= B_0 + B_1 + B_2 > 0\,. \end{aligned} \tag{136}$$

Being $\hat{G}(p; \pi, T)$ a linear function of (p_1, p_2), for fixed p_3, the extremal points of $\hat{G}(p; \pi, T)$ lie necessarily on the boundary of $\bar{\mathcal{S}}$ and can be determined [21] using, for instance, the standard method of Lagrange multipliers. Denoting by $f_A = 0,\ A \in \mathcal{I}_\alpha^{(0)}$ and $f_A > 0,\ A \in \mathcal{I}_\alpha^{(+)}$ the algebraic relations defining the isotropy stratum Σ_α, the conditions one obtains can be written in the following form:

$$\begin{aligned} &\frac{\partial \hat{G}}{\partial p_a} = \sum_{A \in \mathcal{I}_\alpha^{(0)}} \lambda_A \frac{\partial f_A}{\partial p_A} \qquad a = 1, 2, \ldots, q \\ &f_A = 0 \qquad A \in \mathcal{I}_\alpha^{(0)} \\ &f_A > 0 \qquad A \in \mathcal{I}_\alpha^{(+)} \end{aligned} \tag{137}$$

where the λ's are Lagrange multipliers.

The determination of the absolute minimum and of its location(s) is made much easier if one notes that $\hat{G}(p;\pi,T)$ necessarily takes on its absolute minimum in some point of one of the strata $\{O_h\}$, $\{C_{iv}\}$, $i=2,3,4$†, like $C_{\mathrm{as}}(u,v)$ and for the same reasons.

By indexing these strata in the following way:

$$\Sigma_0=\{O_h\} \qquad \Sigma_1=\{C_{4v}\} \qquad \Sigma_2=\{C_{2v}\} \qquad \Sigma_3=\{C_{3v}\} \tag{138}$$

the relations determining the stationary points of the potential can be put in a very compact form.

The relations defining the strata Σ_k, which can be read from table 5, allow us to express p_1 and p_2 in terms of p_3, so that we can define

$$\hat{G}_k(p_3;\pi,T)=\hat{G}(p;\pi,T)\Big|_{\Sigma_k} \qquad k=0\ldots,3\,. \tag{139}$$

Explicitly,

$$\hat{G}_0(0;\pi,T)=0 \tag{140}$$

$$\hat{G}_k(p_3;\pi,T)=p_3\left(\frac{c}{2}+\frac{a_k\,p_3}{4}+\frac{b_k\,p_3^2}{6}\right) \qquad p_3>0 \tag{141}$$

where

$$\left.\begin{aligned} a_k&=A_0+A_1\,k^{-1}\\ b_k&=B_0+B_1\,k^{-1}+B_2\,k^{-2}\end{aligned}\right. \qquad k=1,2,3 \tag{142}$$

and, owing to (136), $b_k>0$.

Now, it is trivial to realize that for $c<0$, each of the functions $\hat{G}_k(p_3;\pi,T)$, $k=1,2,3$ has a local minimum, which is unique and is located at $p_3=p_{3,k}$, where

$$p_{3,k}=\frac{\left(-a_k+\sqrt{a_k^2-4b_kc}\right)}{2b_k}\,. \tag{143}$$

At $p_3=p_{3,k}$, the function $\hat{G}_k(p_3;\pi,T)$ takes on the value:

$$\hat{G}_k^{\min}(\pi,T)=\frac{1}{48b_k^2}\left(a_k-\sqrt{a_k^2-4b_kc}\right)\left(a_k^2-8b_kc-a_k\sqrt{a_k^2-4b_kc}\right) \qquad k=1,2,3\,. \tag{144}$$

For $c\geqslant 0$, the existence of local minima for $\hat{G}_k(p_3;\pi,T)$ depends on the values taken on by A_0 and A_1.

To determine the absolute minimum of $\hat{G}(p;\pi,T)$ and the phase space, one has to compare the values taken on by the functions $\hat{G}_k^{\min}(\pi,T)$.

To be specific, let us restrict our results to the case that $G(x;\pi,T)$ is an expansion in the order parameters of the free-energy of $BaTiO_3$. Following Kim [53], we shall consider the following two possibilities, in which a possible dependence on the pressure π is ignored and CGS units are used:

$$\begin{aligned} c&=7.4(T-110)\times10^{-5}\\ B_0&=0\\ A_0&=1.15\times10^{-12}\\ A_1&=(-0.99-1.15)\times10^{-12}\\ B_1&=0\\ B_2&=0.249\times10^{-21}\end{aligned} \tag{145}$$

† The possibility of a degenerate minimum crossing the strata $\{C_{2v}\}$, $\{C_s'\}$ and $\{C_{4v}\}$ can be excluded by a direct check.

Table 6. Stable phases of $BaTiO_3$ at different temperatures with the first choice for the parameters involved in the definition of the free energy.

Phase	Range of temperatures
$[O_h]$ = cubic	$T > 119.97\ ^\circ\mathrm{C}$
$[O_h],\ [C_{4v}]$	$T = T_{c_1} = 119.97\ ^\circ\mathrm{C}$
$[C_{4v}]$ = tetragonal	$119.97\ ^\circ\mathrm{C} > T > 14.77\ ^\circ\mathrm{C}$
$[C_{4v}],\ [C_{2v}]$	$T = T_{c_2} = 14.77\ ^\circ\mathrm{C}$
$[C_{2v}]$ = orthorhombic	$14.77\ ^\circ\mathrm{C} > T > -87.49\ ^\circ\mathrm{C}$
$[C_{2v}],\ [C_{3v}]$	$T = T_{c_3} = -87.49\ ^\circ\mathrm{C}$
$[C_{3v}]$ = rhombohedral	$-87.49\ ^\circ\mathrm{C} > T$

Table 7. Stable phases of $BaTiO_3$ at different temperatures with the second choice for the parameters involved in the definition of the free energy.

Phase	Range of temperatures
$[O_h]$ = cubic	$T > 115.40\ ^\circ\mathrm{C}$
$[O_h, [C_{4v}]$	$T = T_{c_1} = 115.40\ ^\circ\mathrm{C}$
$[C_{4v}]$ = tetragonal	$115.40\ ^\circ\mathrm{C} > T > -233.52\ ^\circ\mathrm{C}$
$[C_{4v}], [C_{2v}]$	$T = T_{c_2} = -233.52\ ^\circ\mathrm{C}$
$[C_{2v}]$ = orthorhombic	$-233.52\ ^\circ\mathrm{C} > T$

$$
\begin{aligned}
c &= 7.4(T-110)\times 10^{-5}\\
B_0 &= 0\\
A_0 &= 12\times 10^{-13}\\
A_1 &= 4\times 4.5(T-175)\times 10^{-15} - 12\times 10^{-13}\\
B_1 &= 24\times 10^{-23}\\
B_2 &= 30\times 10^{-23}\,.
\end{aligned}
\tag{146}
$$

Then, using the data specified in (145), for $T > 119.97\ ^\circ$C, the free energy takes on its absolute minimum at Σ_0; thus only the disordered cubic phase $[O_h]$ is stable at these temperatures. At $T = 119.97\ ^\circ$C, the function $\hat{G}_1^{\min}(T)$ vanishes, so that the cubic and tetragonal phases coexist. For $119.97\ ^\circ\mathrm{C} < T < 14.77$ the absolute minimum sits on $\{C_{4v}\}$ and the tetragonal phase $[_4v]$ is stable. At $T = 14.77\ ^\circ$C, the absolute minimum shifts to $\{C_{2v}\}$ and for $14.77\ ^\circ\mathrm{C} < T < -87.49$ the stable phase is the orthorhombic one. At $T = -87.49$ the absolute minimum shifts to $\{C_{3v}\}$ and for $T < -87.49$ the stable phase is the rhombohedral one.

These results, and the analogous ones obtained using the data specified in (146), of (146), are resumed in tables 6 and 7.

If the free energy is expanded as a sufficiently high degree polynomial in the order parameters x, and for a convenient choice of the coefficients as functions of T, all the phases represented by the isotropy type strata of the orbit space of O_h may become accessible (as stable phases) to the system at convenient temperatures. In particular, the sub-principal strata require at least an 8th-degree polynomial, while the principal stratum requires at least a 12th-degree polynomial.

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